Implementation of analysis-suitable parameterization construction using G+Smo

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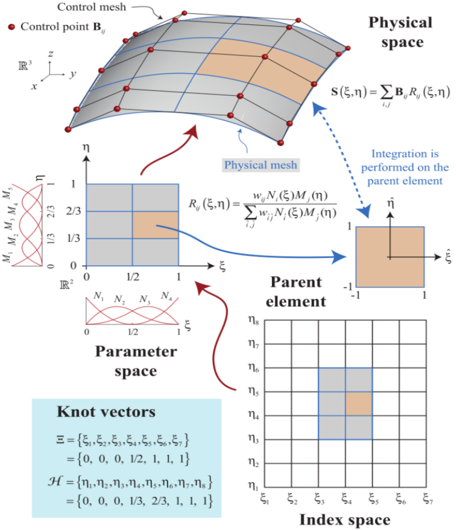
Contributors

- Ye Ji et al., Constructing high-quality planar NURBS parameterization for isogeometric analysis by adjustment control points and weights, Journal of Computational and Applied Mathematics, 396 (2021), 113615.
- Ye Ji et al., Penalty function-based volumetric parameterization method for isogeometric analysis, Computer Aided Geometric Design, 94 (2022), 102075.

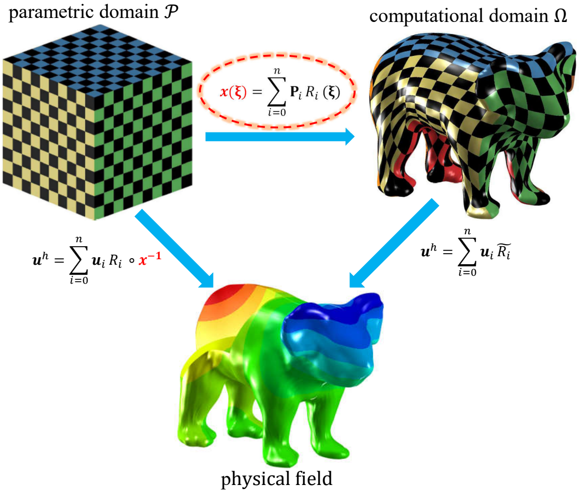
IsoGeometric Analysis (IGA)



Source: Figure from [Cottrell et al. 2009]

- Proposed by T.J.R. Hughes et al., 2005.
- **KEY IDEA:** approximate the physical fields with the same basis functions as that used to generate CAD models.
- Advantages:
  - Integration of design and analysis;
  - Exact and efficient geometry;
  - No data type transition and mesh generation;
  - Simplified mesh refinement;
  - High order continuous field;
  - Superior approximation properties.
- Very broad applications: such as shell analysis, fluid-structure interaction, and shape and topology optimization.

Research motivation



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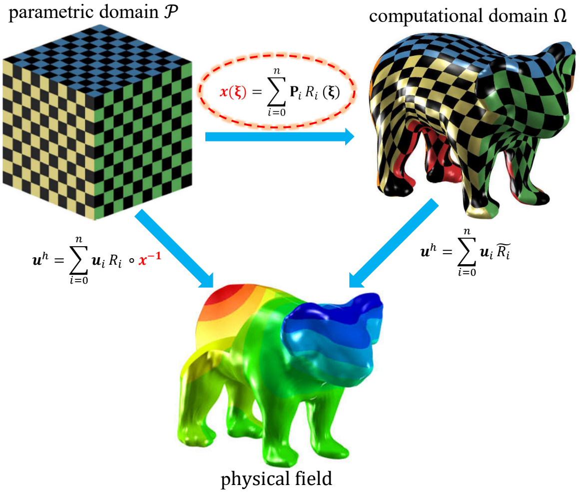

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- **Problem statement**:
  - From a given B-Rep, constructing an analysis-suitable parameterization $\boldsymbol{x}$.

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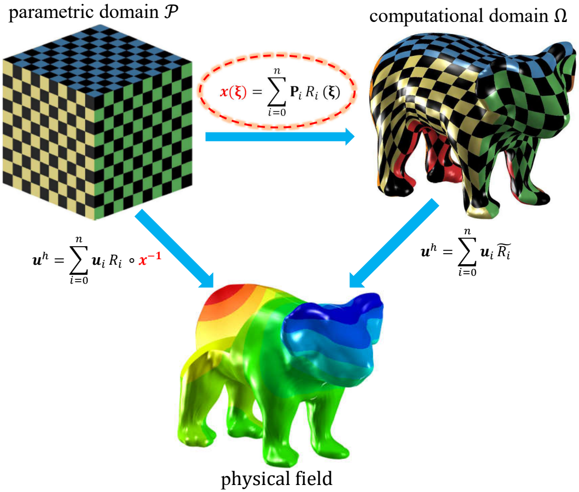


- Most modern CAD systems only focus on boundary representations (B-Reps) in geometry modeling.
- **Problem statement**:
  - From a given B-Rep, constructing an analysis-suitable parameterization x.
  - Analysis-suitable parameterizations should
    - be **bijective**;
    - ensure as **low angle and volume distortion** as possible.

Problem statement

- A spline-based parameterization $\boldsymbol{x}$ from a parametric domain $\mathcal{P} = [0,1]^d$ $(d = 2,3)$ to computational domain Ω is of the following form

$$\boldsymbol{x}(\boldsymbol{\xi}) = \mathbf{R}^{\mathrm{T}}\mathbf{P} = \underbrace{\sum_{i \in \mathcal{I}_I} \mathbf{P}_i R_i(\boldsymbol{\xi})}_{\text{unknown}} + \underbrace{\sum_{j \in \mathcal{I}_B} \mathbf{P}_j R_j(\boldsymbol{\xi})}_{\text{known}}, \tag{1}$$

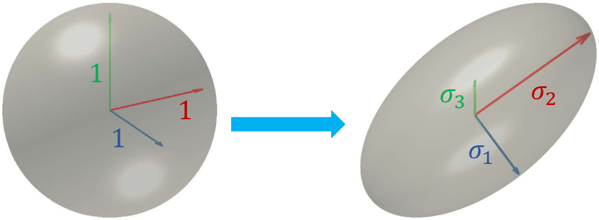
  where $\mathbf{P}_i$ are unknown inner control points and $\mathbf{P}_j$ are given boundary control points.
- **GOAL:** To construct the **unknown inner control points $\mathbf{P}_i$** such that $\boldsymbol{x}$ is **bijective** and has the **lowest possible angle and area/volume distortion**.

Objective function: angle distortion

- Most-Isometric ParameterizationS (MIPS) energy [Hormann and Greiner 2000, Fu et al. 2015]:

$$E_{\text{angle}}(\boldsymbol{x}) = \begin{cases} \frac{\sigma_1}{\sigma_2} + \frac{\sigma_2}{\sigma_1}, & 2D, \\ \frac{1}{8}\left(\frac{\sigma_1}{\sigma_2} + \frac{\sigma_2}{\sigma_1}\right)\left(\frac{\sigma_2}{\sigma_3} + \frac{\sigma_3}{\sigma_2}\right)\left(\frac{\sigma_1}{\sigma_3} + \frac{\sigma_3}{\sigma_1}\right), & 3D. \end{cases} \tag{2}$$

  where σ_i are the singular values of the Jacobian matrix $\mathcal{J}$ of the parameterization $\boldsymbol{x}$.
- When $\sigma_1 = \sigma_2 = \ldots = \sigma_d$, $\boldsymbol{x}$ is conformal and E_{angle} reaches its minimum value.

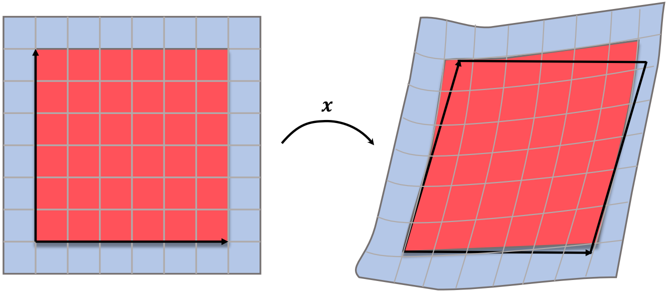


Objective function: area/volume distortion

- Area/volume distortion energy:

$$E_{\mathrm{vol}}(\boldsymbol{x}) = \frac{|\mathcal{J}|}{vol(\Omega)} + \frac{vol(\Omega)}{|\mathcal{J}|}, \tag{3}$$

where $vol(\Omega)$ denotes the area/volume of the computational domain Ω;



Objective function: variational formulation

- **Basic idea**: to solve the following constrained optimization problem:

$$\begin{aligned} \underset{\mathbf{P}_i,\ i\in\mathcal{I}_I}{\arg\min} \quad & E(\boldsymbol{x}) = \int_{\mathcal{P}} \left(\lambda_1 E_{\text{angle}}(\boldsymbol{x}) \ + \lambda_2 E_{\text{vol}}(\boldsymbol{x})\right) \,\mathrm{d}\mathcal{P}, \\ s.t. \quad & \boldsymbol{x} \text{ is bijective.} \end{aligned} \tag{4}$$

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- Suppose that the given B-Rep is bijective. $\boldsymbol{x}$ is bijective $\Leftrightarrow |\mathcal{J}(\boldsymbol{x}(\boldsymbol{\xi}))| \neq 0,\ \forall \boldsymbol{\xi} \in \mathcal{P}$.

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- Suppose that the given B-Rep is bijective. $\boldsymbol{x}$ is bijective $\Leftrightarrow |\mathcal{J}(\boldsymbol{x}(\boldsymbol{\xi}))| \neq 0, \ \forall \boldsymbol{\xi} \in \mathcal{P}$.
- Due to the high-order continuity of $\boldsymbol{x}$, we need $|\mathcal{J}| > 0 \ (< 0), \ \forall \boldsymbol{\xi} \in \mathcal{P}$.

Treatment of bijectivity constraint

- The Jacobian determinant can be represented by a linear combination of splines

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- However, the number of the constraints can be huge. [Pan et al., CMAME 2020, Ji et al. JCAM 2021]. (To a bi-cubic planar NURBS parameterization with 20×20 control points, the number of inequality constraints is over 34**k**.)

Equivalence problem: unconstrained optimization

- Recall the planar MIPS energy,

$$E^{2D}_{angle}(\boldsymbol{x}) = \frac{\sigma_1^2 + \sigma_2^2}{\sigma_1 \sigma_2} = \frac{trace(\mathcal{J}^{\mathrm{T}}\mathcal{J})}{|\mathcal{J}|}.$$

Since the Jacobian determinant appears in its denominator, it proceeds to infinity if the Jacobian determinant $|\mathcal{J}|$ approaches zero.

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  Since the Jacobian determinant appears in its denominator, it proceeds to infinity if the Jacobian determinant $|\mathcal{J}|$ approaches zero.

- Remove the constraints and solve the following **unconstrained optimization problem**:

$$\underset{\mathbf{P}_i,\ i\in\mathcal{I}_I}{\arg\min} \quad E(\boldsymbol{x}) = \int_{\mathcal{P}} \left(\lambda_1 E_{\text{angle}}(\boldsymbol{x}) \ + \lambda_2 E_{\text{vol}}(\boldsymbol{x})\right) \ \mathrm{d}\mathcal{P}. \tag{6}$$

Hybrid L-BFGS (HLBFGS) solver (NEW in G+Smo!)

(https://xueyuhanlang.github.io/software/HLBFGS/)

- A framework for unconstrained optimization problems written by Yang Liu (Microsoft Research Asia).
  - Light-weight and freely available for non-commercial purposes;
  - Unifies common optimization methods, such as gradient-decent method, (Preconditioned) L-BFGS method, (Preconditioned) Conjugate Gradient method, and Newton's method.
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  - Very popular in computer graphics community.
- Already integrated into G+Smo (stable):
  - Example: examples/optimizer_example.cpp;
  - G+Smo wrapper: /extensions/gsHLBFGS/gsHLBFGS.h;
  - Source codes: /external/HLBFGS.

Basic usage of HLBFGS solver (NEW in G+Smo!)

```
template <typename T>
class gsOptProblemExample : public gsOptProblem<T> {
public:
    // The constructor defines all properties of our optimization problem
    gsOptProblemExample() {};

    // The evaluation of the objective function must be implemented
    T evalObj(const gsAsConstVector<T> &u) const {};

    // The gradient (resorts to finite differences if unimplemented)
    void gradObj_into(const gsAsConstVector<T> &u, gsAsVector<T> &result) const {};
    ...
}
```

Basic usage of HLBFGS solver (NEW in G+Smo!)

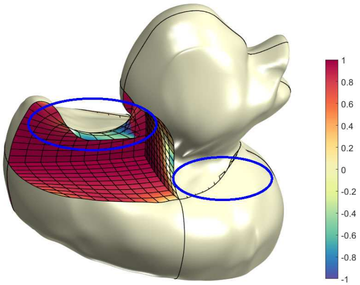
```
int main(int argc, char* argv[]){
    ...
    gsOptProblemExample<real_t> problem;
    gsHLBFGS<real_t> *optimizer;

    // Set stopping criterion for iteration (optional)
    optimizer->options().setInt("MaxIterations", 200);
    optimizer->options().setInt(...);

    // Set initial guess (optional)
    gsVector<real_t> initialGuess;
    initialGuess << ...;

    // Solve
    optimizer->solve(initialGuess);
    ...
}
```

Initialization

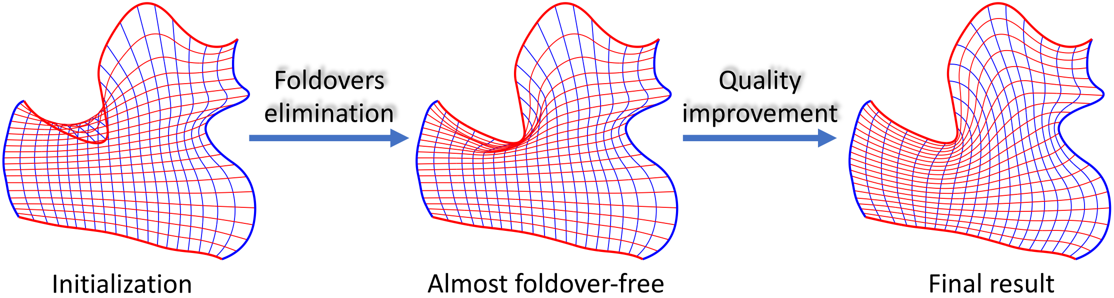


Initial parameterization.

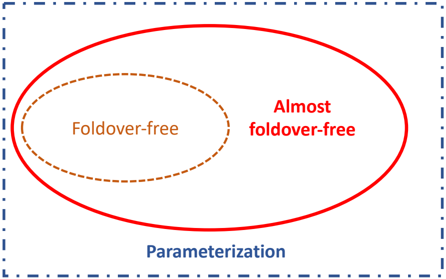
- Many algebraic methods can be adopted to initialize:
  - Discrete Coon's patch [Farin and Hansford 1999];
  - Spring patch [Gravesen et al. 2012];
  - Smoothness energy minimization [Wang et al. 2003, Pan et al. 2020];
  - ...
- No guarantee of bijectivity.
- However, an already bijective parameterization is needed in our optimization problem (6).

Barrier function-based parameterization construction

- Three-step strategy.



Foldovers elimination: almost foldover-free parameterization

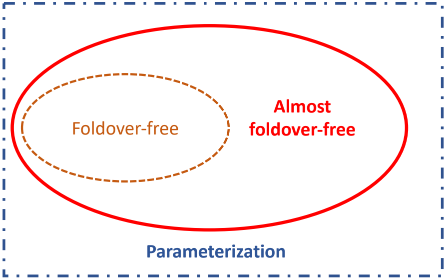


- Some works solve the following Max-Min problem:

$$\underset{\mathbf{P}_i,\ i\in\mathcal{I}_I}{\arg\min}\ \max_j\ |\mathcal{J}|_j\ ,$$

where $|\mathcal{J}|_j$ are the expansion coefficients of $|\mathcal{J}|$.
- **High computational costs still but NOT necessary!**

Foldovers elimination: almost foldover-free parameterization



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where $|\mathcal{J}|_j$ are the expansion coefficients of $|\mathcal{J}|$.

- **High computational costs still but NOT necessary!**
- We solve the following problem instead:

$$\underset{\mathbf{P}_i,\ i\in\mathcal{I}_I}{\arg\min}\quad E(\boldsymbol{x}) = \int_{\mathcal{P}} \max\left(0, \delta - |\mathcal{J}|\right)\, \mathrm{d}\mathcal{P},$$

where δ is a threshold ($\delta = 5\% vol(\Omega)$ as default).

Foldovers elimination: almost foldover-free parameterization

gsObjFoldoverFree

```cpp
template<short_t d, typename T>
T gsObjFoldoverFree<d, T>::evalObj(const gsAsConstVector<T> &u) const
{
    // update m_mp with the current design
    convert_gsFreeVec_to_mp<T>(u, m_mapper, m_mp);
    geometryMap G = m_evaluator.getMap(m_mp);

    // defines the expression of integrand
    auto EfoldoverFree = (m_delta - jac(G).det()).ppartval();
    return m_evaluator.integral(EfoldoverFree);
}
```

Foldovers elimination: almost foldover-free parameterization

- Foldovers elimination is of vital importance. If it fails, everything **CRASHES!!!**
- For practical purposes, we gradually reduce the δ.

```
...
gsObjFoldoverFree<d, T> objFoldoverFree(mp, mapper);
do {
    T delta = pow(0.1, it) * 5e-2 * scaledArea; // update the parameter delta
    objFoldoverFree.options().setReal("ff_Delta", delta);
    objFoldoverFree.applyOptions();

    gsHLBFGS<T> optFoldoverFree(&objFoldoverFree);
    optFoldoverFree.solve(initialGuessVector); // solve the current problem

    Efoldover = optFoldoverFree.currentObjValue();
    initialGuessVector = optFoldoverFree.currentDesign();
    ++it;
} while (Efoldover > 1e-20 && it < 10);
```

Quality improvement: robustness consideration

- Recall that E_{angle} proceeds to infinity if the Jacobian determinant $\mathcal{J}$ approaches zero.
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Quality improvement: robustness consideration

- Recall that E_{angle} proceeds to infinity if the Jacobian determinant $\mathcal{J}$ approaches zero.
- DANGER!: discontinuous function value change in numerical optimization.
- Line search ensures sufficient reduction, e.g., strong Wolfe condition.
- With this feature, we simply revise the objective function (barrier function):

$$E^c = \begin{cases} \int_{\mathcal{P}} \left(\lambda_1 E_{\text{angle}}(\boldsymbol{x}) + \lambda_2 E_{\text{vol}}(\boldsymbol{x})\right) \, \mathrm{d}\mathcal{P}, & \text{if } \min|\mathcal{J}| > 0, \\ +\infty, & \text{otherwise.} \end{cases}$$

Quality improvement

```cpp
template<short_t d, typename T>
template<short_t _d>
typename std::enable_if<_d == 2, T>::type
gsObjQualityImprovePt<d, T>::evalObj(const gsAsConstVector<T> &u) const
{
    // update m_mp with the current design
    ...

    // set the objective function value to +\infty if min(jac(G).det()) < 0
    if (m_evaluator.min(jac(G).det()) < 0){return std::numeric_limits<T>::max();}
    else {
        // otherwise, compute the normal objective function value
        auto Euniform = chi / area + area / chi;;
        auto Ewinslow = jac(G).sqNorm() / jac(G).det();
        return m_evaluator.integral(m_lambda1 * Ewinslow + m_lambda2 * Euniform);
    }
}
```

Analytical gradient: for stability aspect

- In the class `gsOptProblem<T>`, we have a default `gradObj_into()` which approximate the gradient by numerical differentiation

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x+2h)}{12h} + \frac{h^4}{30} f^{(5)}(c),$$

where $c \in [x-2h, x+2h]$.

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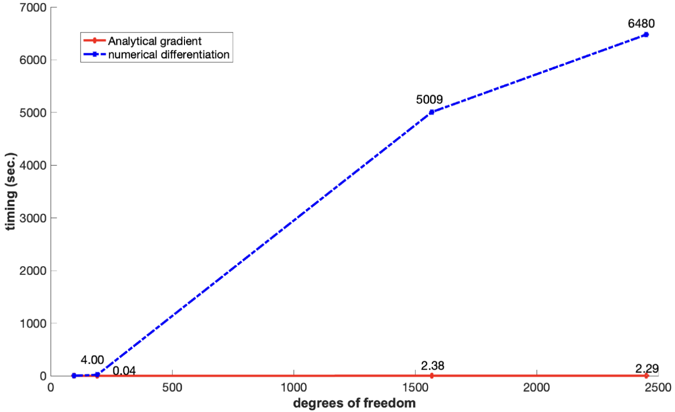
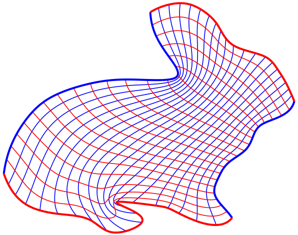
  where $c \in [x-2h, x+2h]$.
- Hard to select a suitable step size h, especically for our problem.

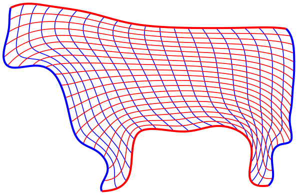
Analytical gradient: for efficiency aspect

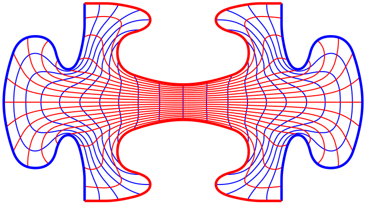
- To a single-patch tri-cubic B-spline parameterization with 25 control points along each direction (using standard Gauss quadrature rule), $4 * 23^3 * (3+1)^3 > 3$ M function evaluations are performed for once line-search.

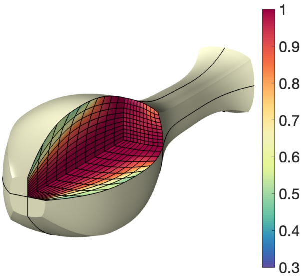


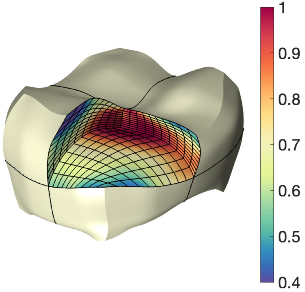
Gallery: barrier function-based method

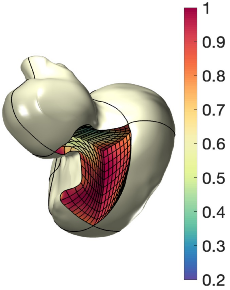












Penalty function-based parameterization construction

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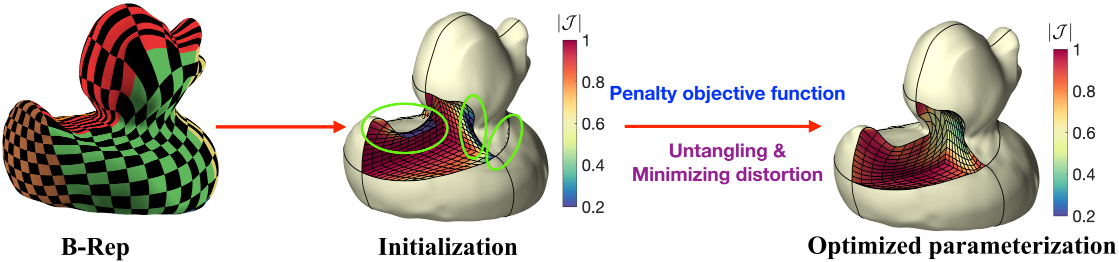
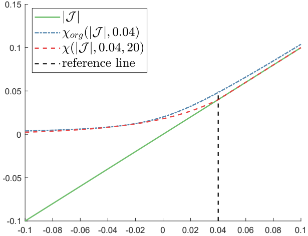
Penalty function-based parameterization construction

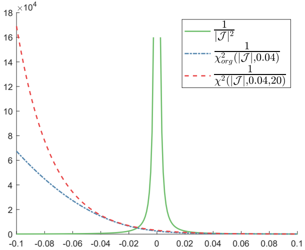
- The foldovers elimination does not improve sufficient to the parameterization quality.
- Avoids extra foldovers elimination steps.
- **Untangling and minimizing distortion perform simultaneously!!!**



Basic idea: Penalty function



$\chi(|\mathcal{J}|, \varepsilon, \beta)$



$\frac{1}{\chi^2(|\mathcal{J}|,\varepsilon,\beta)}$

- **Penalty function:**

$$\chi(|\mathcal{J}|, \varepsilon, \beta) = \begin{cases} \varepsilon \cdot e^{\beta(|\mathcal{J}|-\varepsilon)} & \text{if } |\mathcal{J}| \leq \varepsilon \\ |\mathcal{J}| & \text{if } |\mathcal{J}| > \varepsilon \end{cases}, \tag{7}$$

where ε is a small positive number and β is a penalty factor;

- $\chi(|\mathcal{J}|, \varepsilon, \beta)$ equals a small positive number if $|\mathcal{J}| < \varepsilon$, and strictly equals the Jacobian determinant $|\mathcal{J}|$ if $|\mathcal{J}| \geq \varepsilon$;

- $\frac{1}{\chi^2(|\mathcal{J}|,\varepsilon,\beta)}$ have **very large values to penalize the negative Jacobians and small values to accept positive Jacobians**.

Jacobian regularization and revised objective function

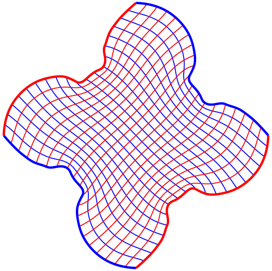
- With this basic idea, we solve the following optimization problem:

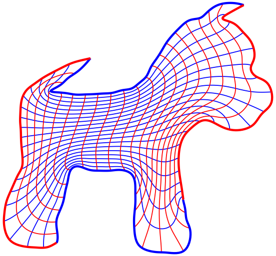
$$\begin{aligned}\underset{\mathbf{P}_i,\ i\in\mathcal{I}_I}{\arg\min}\, E^c &= \int_{\mathcal{P}} \left(\lambda_1 E^c_{\text{mips}} + \lambda_2 E^c_{\text{vol}}\right)\, \mathrm{d}\mathcal{P} \\ &= \int_{\mathcal{P}} \left(\frac{\lambda_1}{8}\kappa_F^2(\boldsymbol{\mathcal{J}}) \cdot \frac{|\boldsymbol{\mathcal{J}}|^2}{\chi^2(|\boldsymbol{\mathcal{J}}|,\varepsilon,\beta)} + \lambda_2\left(\frac{vol(\Omega)}{\chi(|\boldsymbol{\mathcal{J}}|,\varepsilon,\beta)} + \frac{\chi(|\boldsymbol{\mathcal{J}}|,\varepsilon,\beta)}{vol(\Omega)}\right)\right)\, \mathrm{d}\mathcal{P},\end{aligned} \tag{8}$$

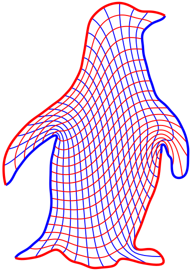
where $\mathbf{P}_i,\ i\in\mathcal{I}_I$ are the unknown inner control points.

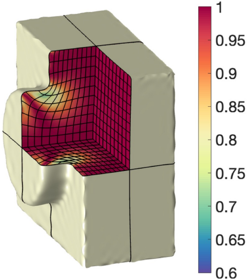
- Now, **only one optimization problem is solved.**

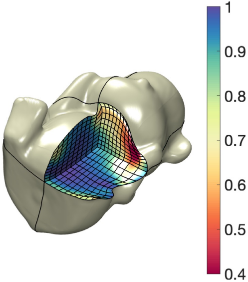
Gallery: penalty function-based results

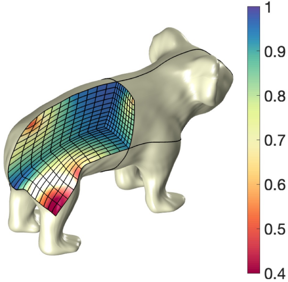




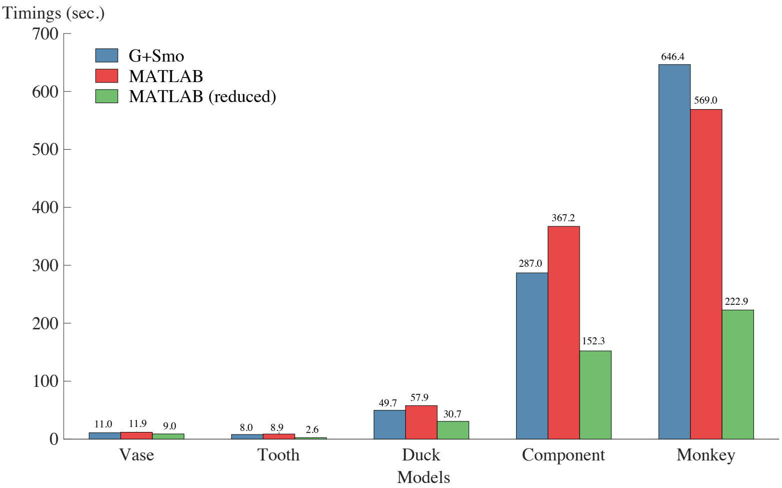






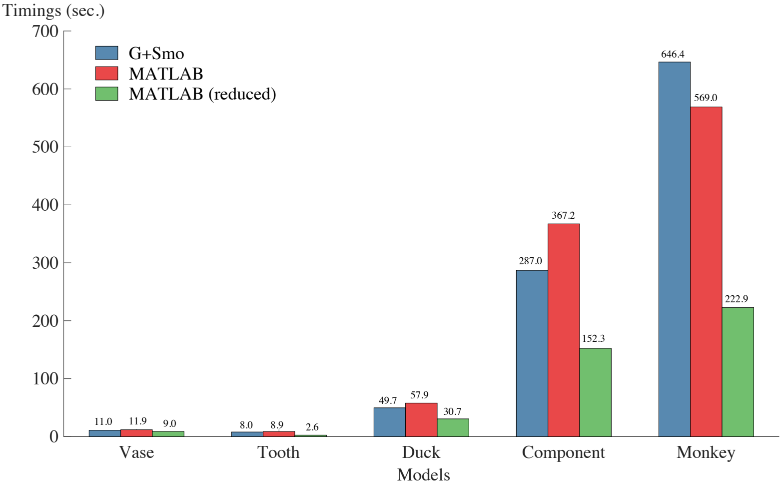


Timing comparisons of G+Smo and MATLAB implementations



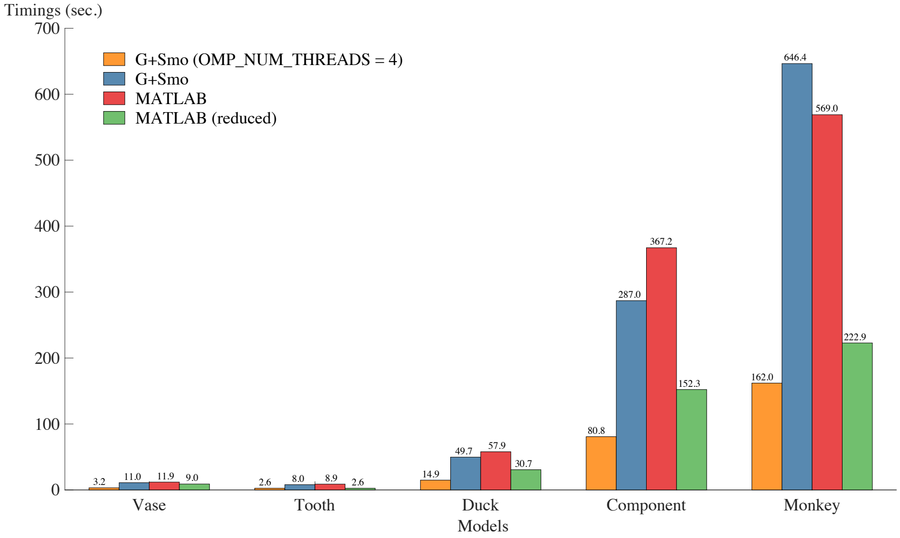
- G+Smo code is not as fast as we expected.

Timing comparisons of G+Smo and MATLAB implementations

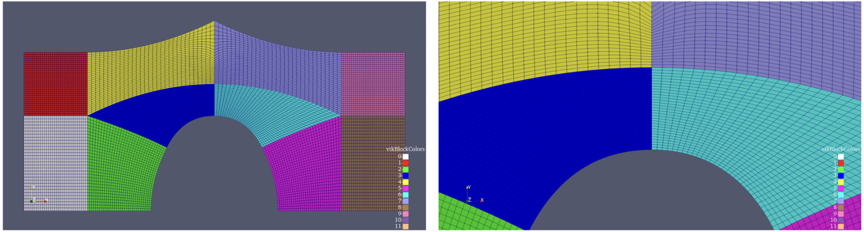


- G+Smo code is not as fast as we expected.
- Precompute basis functions (unsteady problems and structural optimization).

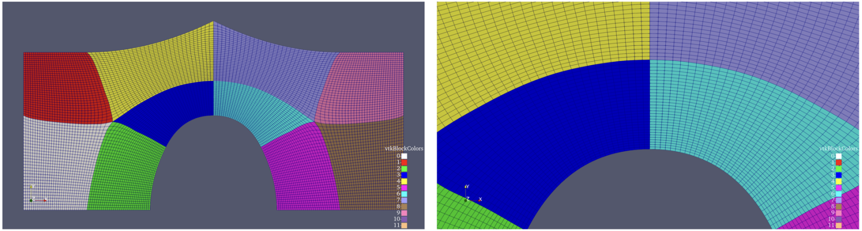
G+Smo implementation with OPENMP



Multi-patch result: `multipatch_tunnel.xml`

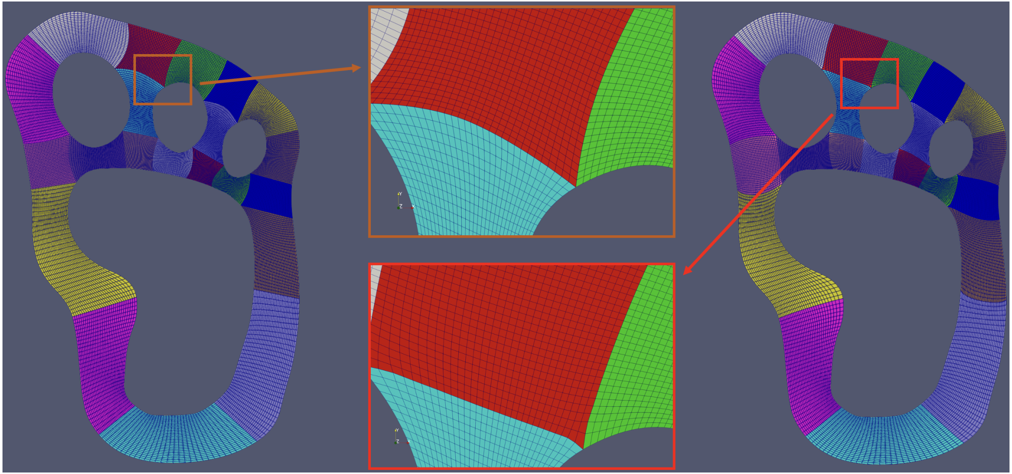


Fixed interfaces

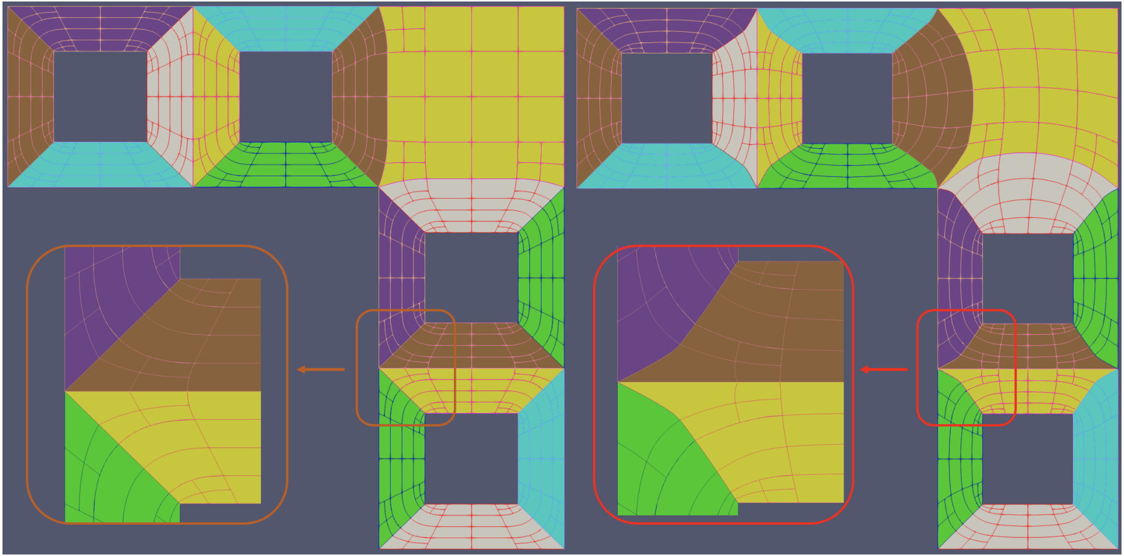


Free interfaces

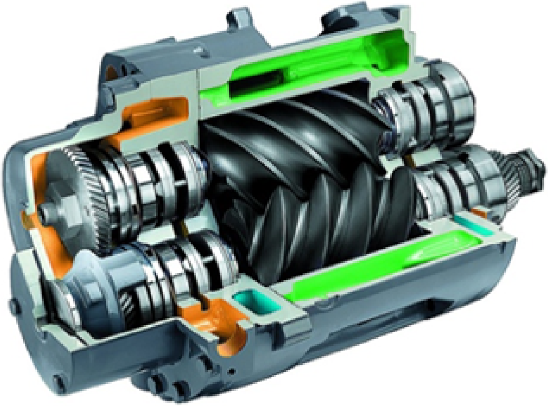
Multi-patch result: `yeti_footprint.xml`

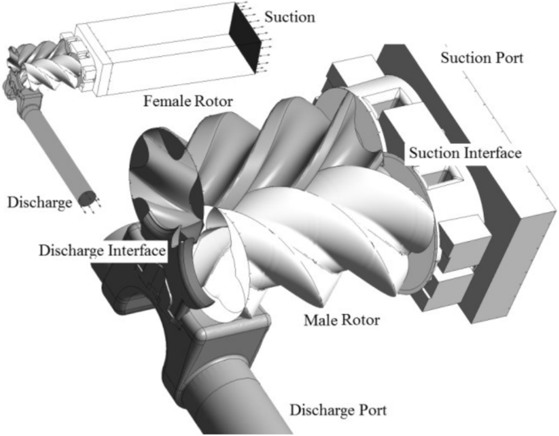


Compatible to multi-patch THB parameterization

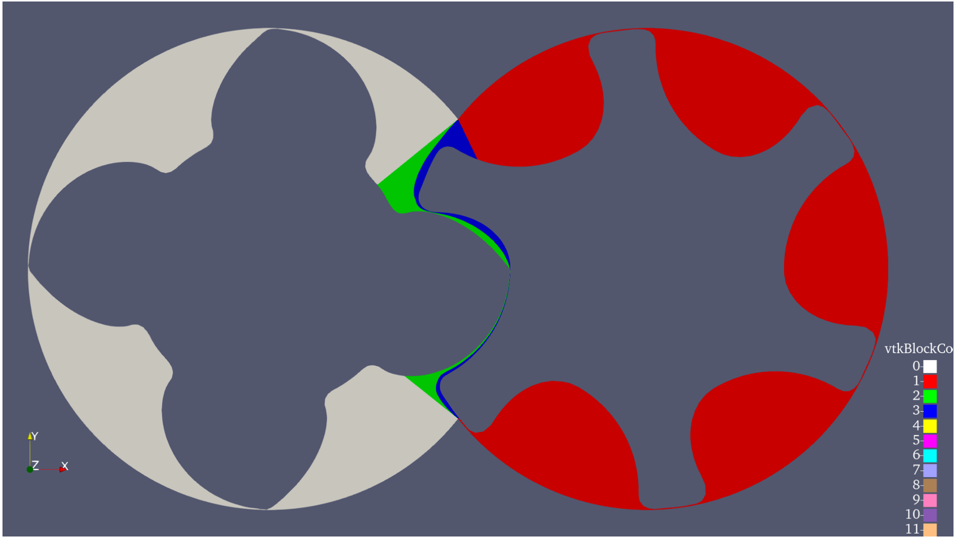


Application: twin-screw rotary compressor

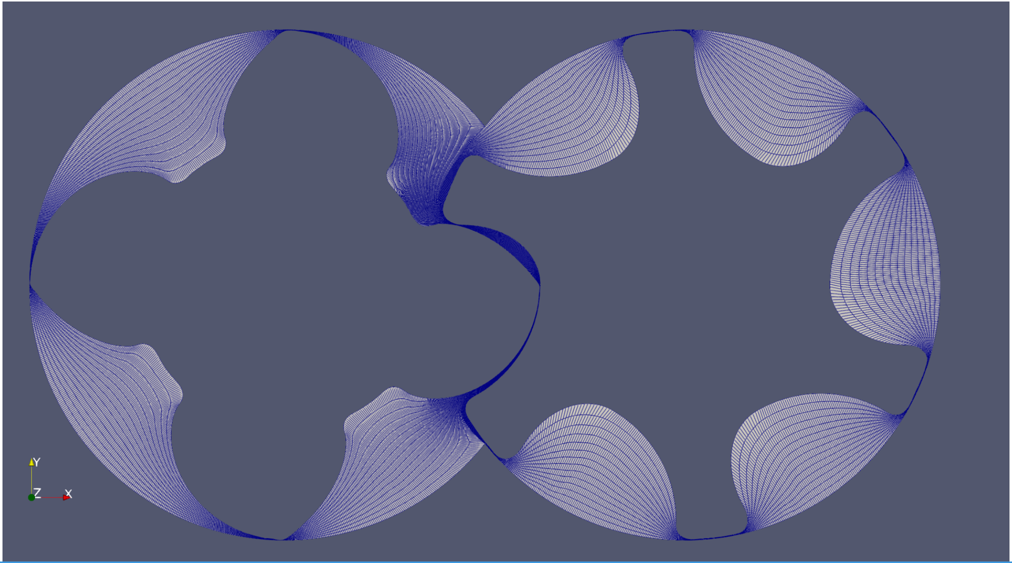




Application: twin-screw rotary compressor



Application: twin-screw rotary compressor



Thanks for your attention!

Q&A.

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