

Multiscale isogeometric fracture simulation

XFEM, IGA, Embedded interfaces, digital twins

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Computational mechanics & computational materials sciences

Multiscale/field interface problems

COMPETENCES

DISCRETISATION

discrete and continuum approaches

MULTI-SCALE FRACTURE

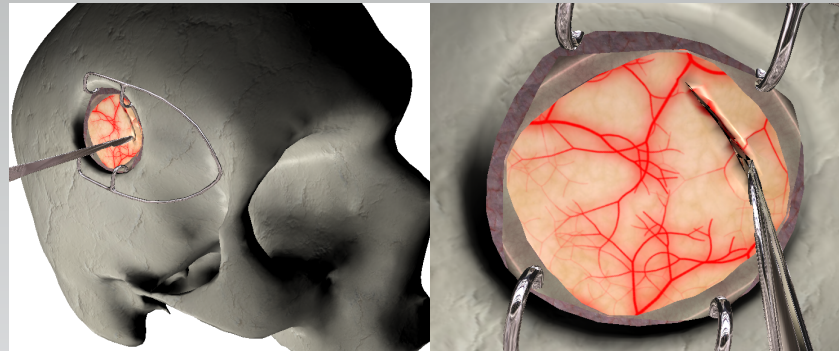
aerospace composites, polycrystalline materials

COUPLED PROBLEMS

biofilms, liquid crystals, fluid-structure, batteries

QUALITY & ERROR CONTROL

optimise computational time given an accuracy level



Real-time simulation of cutting during brain surgery

INTERACTIVITY

Reduce computational costs by several orders of magnitude

APPLICATIONS

PERSONALISED MEDICINE

Computer-aided surgery

Computer-aided diagnostics

ENGINEERING

Durability & Sustainability

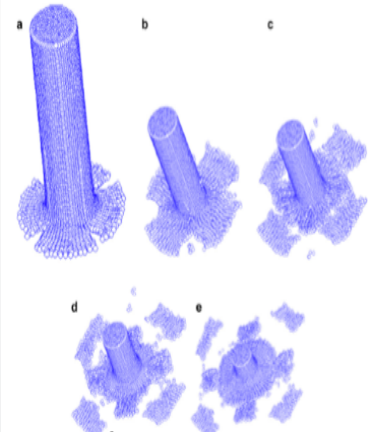
Energy

Aerospace

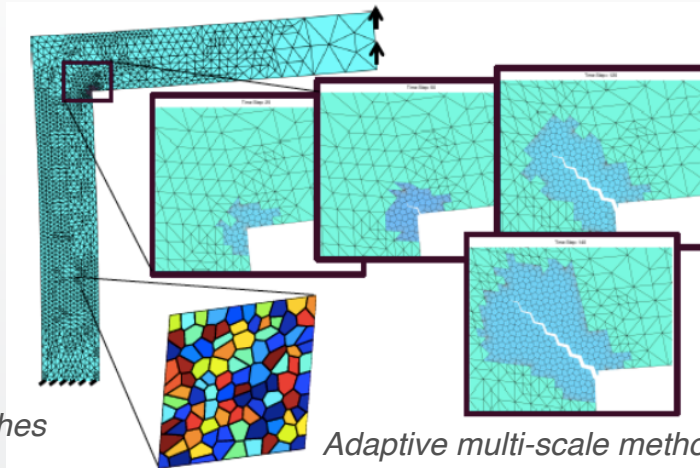
Discretisation

Fracture over multiple scales

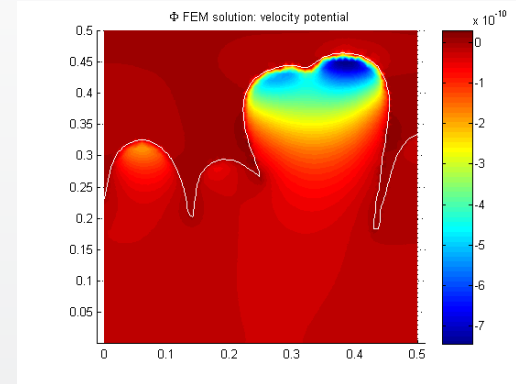
Coupled problems



Mesh-free and discrete approaches to fracture



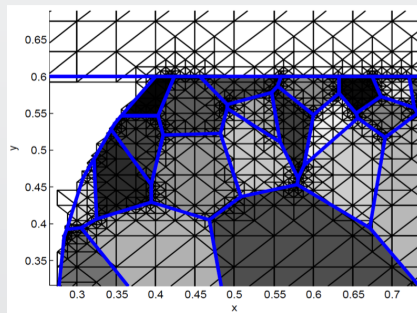
Adaptive multi-scale methods



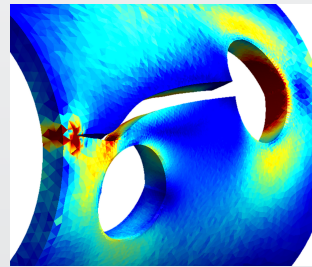
Biofilm growth

Quality and error control

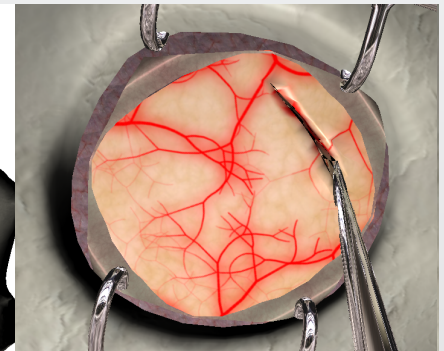
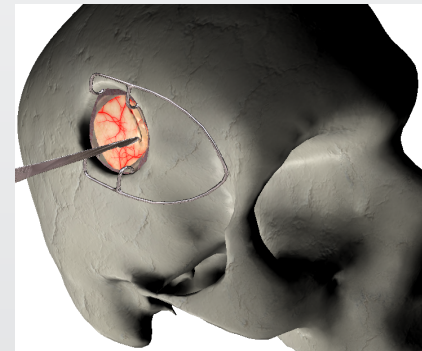
Interactivity and model order reduction



Durability of Pb-free solders



Error estimates for fracture



APPLICATIONS

Personalised Medicine

Engineering

Computer-aided surgery

Computer-aided diagnostics

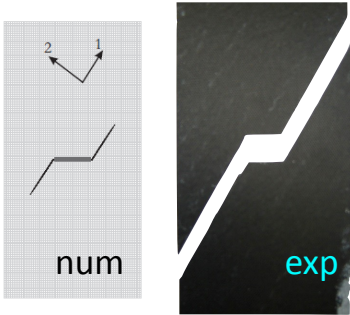
Durability & Sustainability

Energy

Aerospace

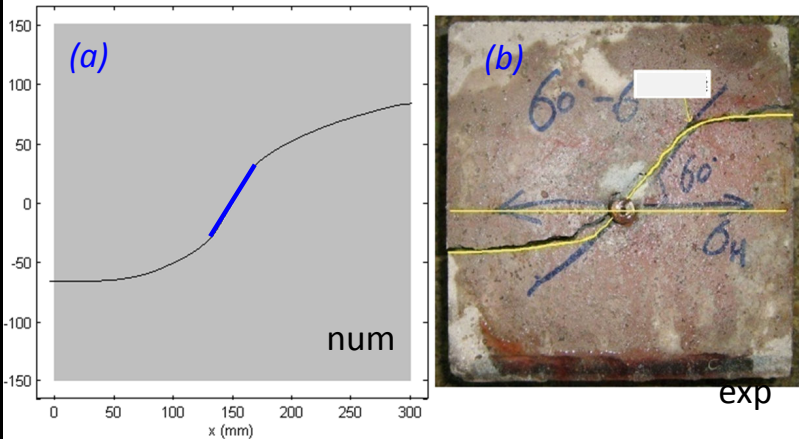
Motivation: fracture of engineering structures and materials

► Limerick: unidirectional composites

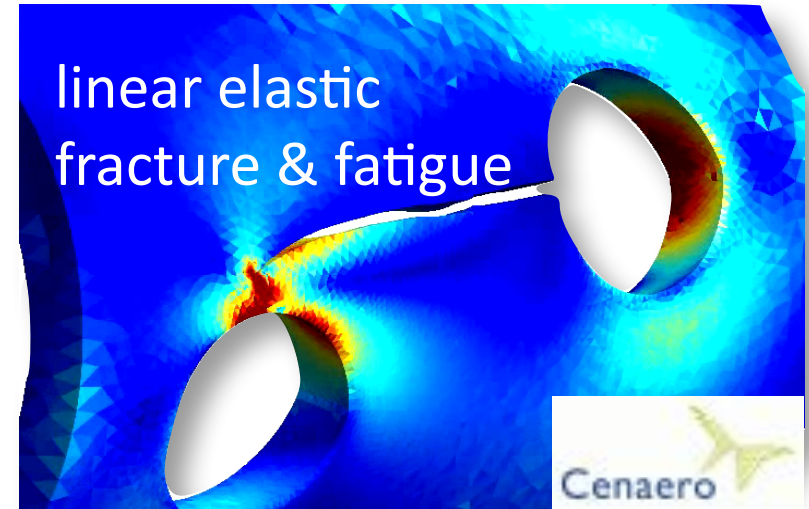


thesis L. Cahill,
2014

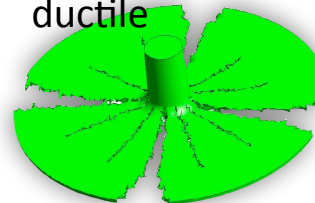
► China/USA: hydraulic fracturing (shale gas)



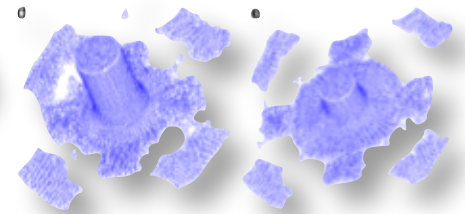
thesis M. Sheng, USA, China, 2016



dynamics
ductile

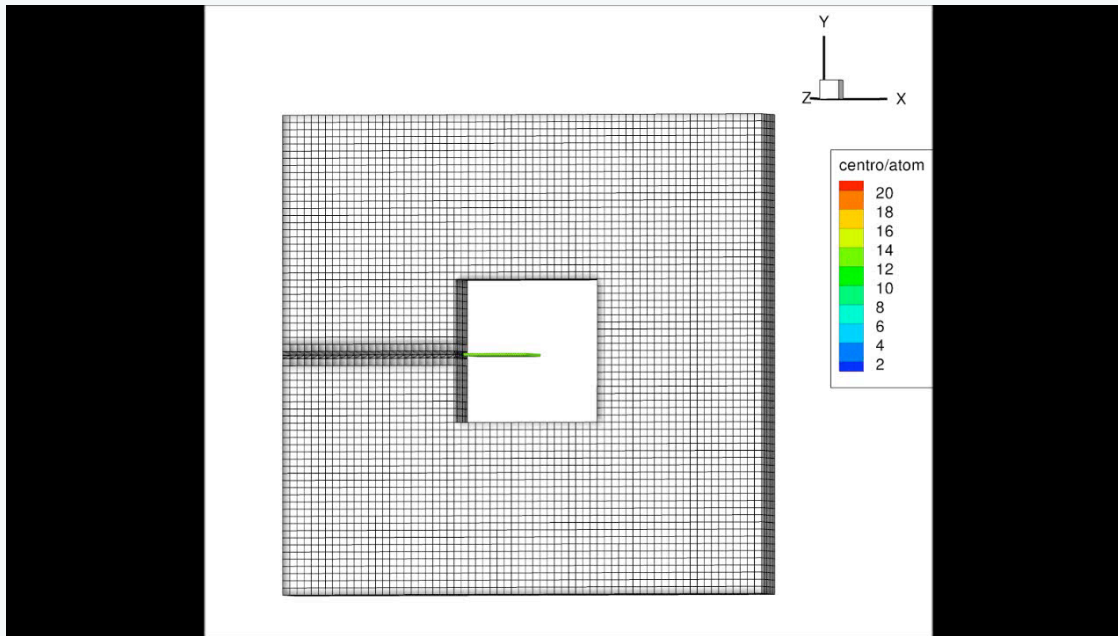
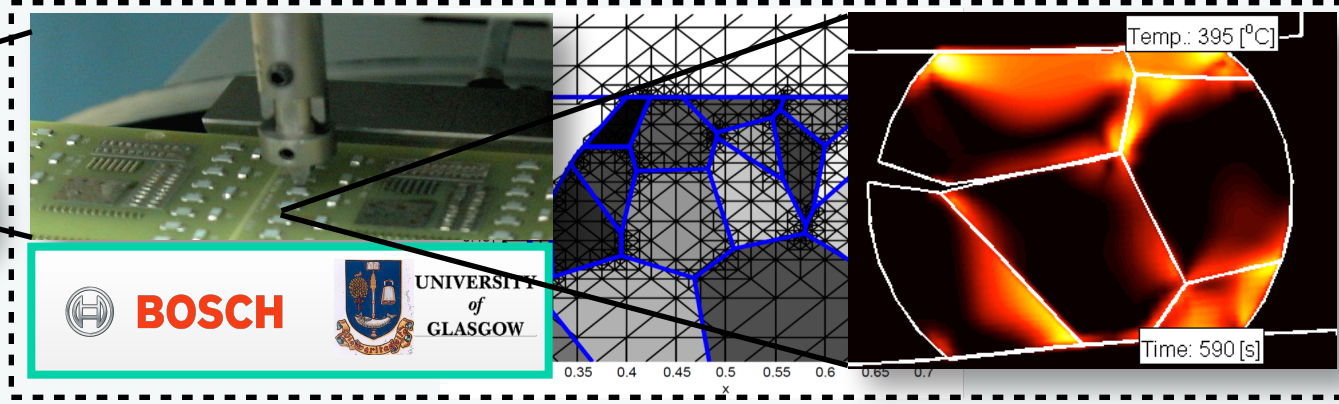
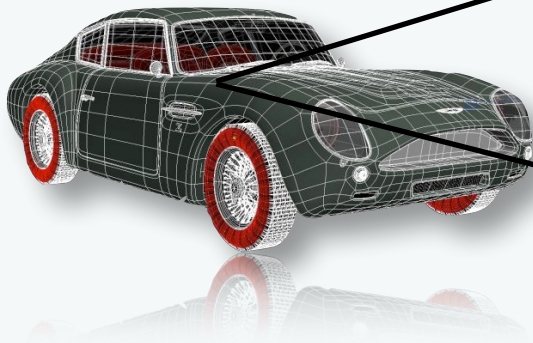


dynamics/brittle



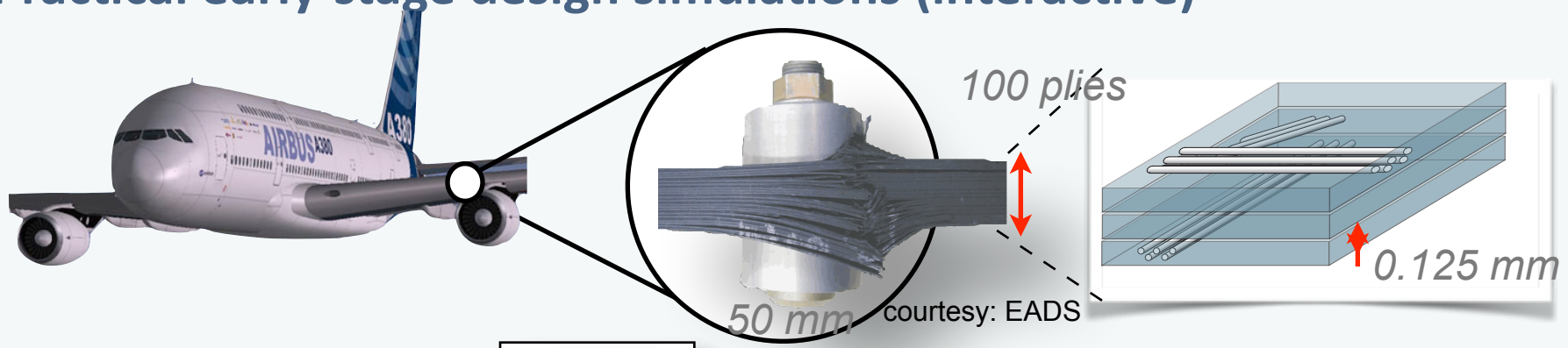
Motivation: multiscale fracture of engineering structures and materials

Solder joint durability (microelectronics), Bosch GmbH

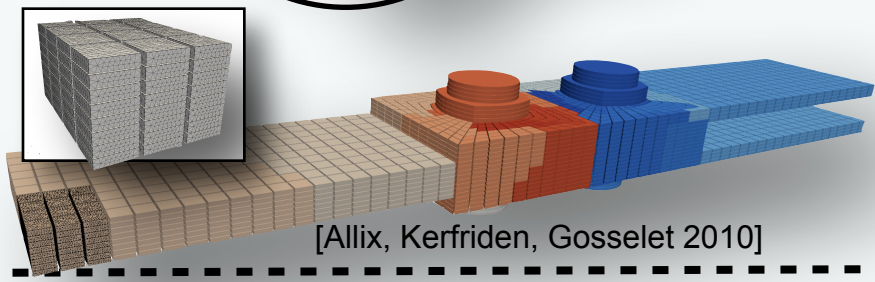


Motivation: multiscale fracture of engineering structures and materials

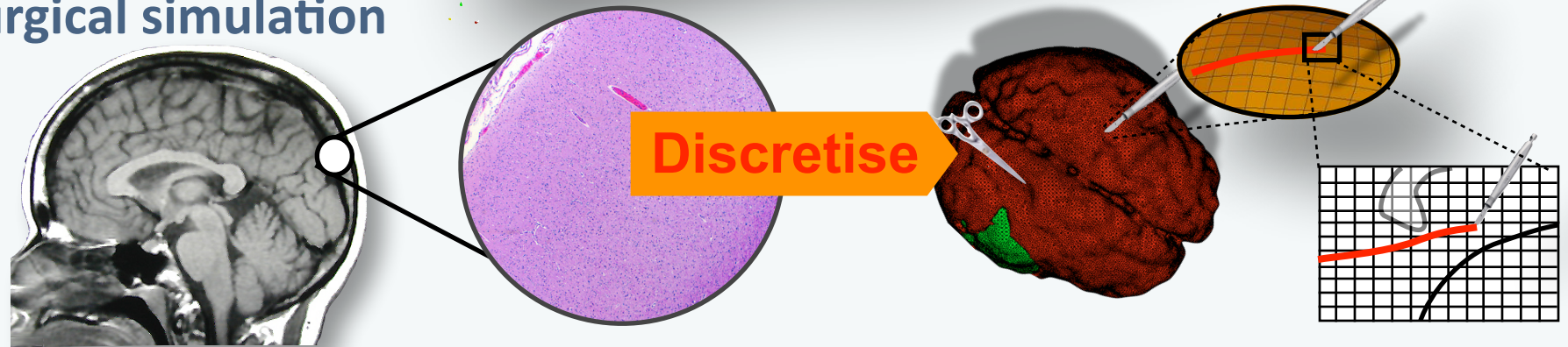
Practical early-stage design simulations (interactive)



Discretise

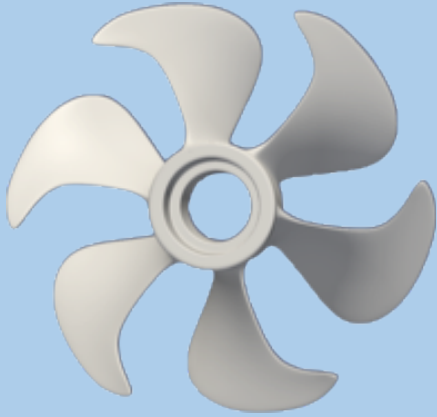


Surgical simulation

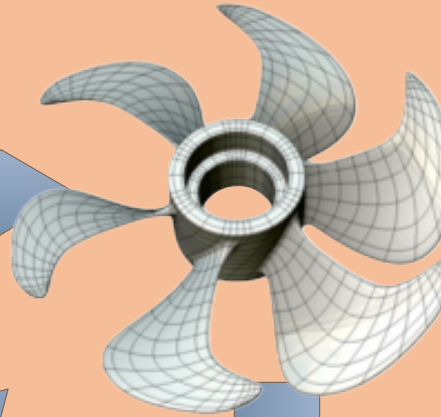


- ▶ Reduce the problem size while controlling the error (in QoI) when solving very large (multiscale) mechanics problems

GEOMETRICAL MODEL



DISCRETISATION



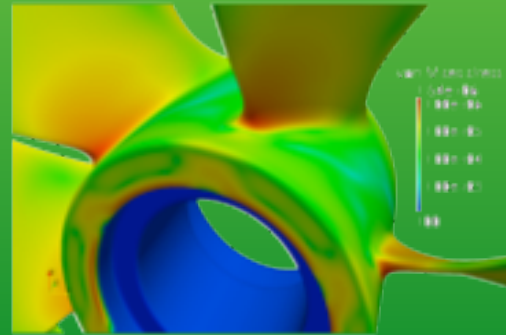
Verification

MATERIAL MODELS

Phenomenological
Elasticity/Plasticity
Crack growth law (Paris...)
Fracture energy
Maximum tensile strength

Multi-scale
Debonding, Fibre pull-out
Fibre breakage, interface
fracture, grains,

NUMERICAL SOLUTION



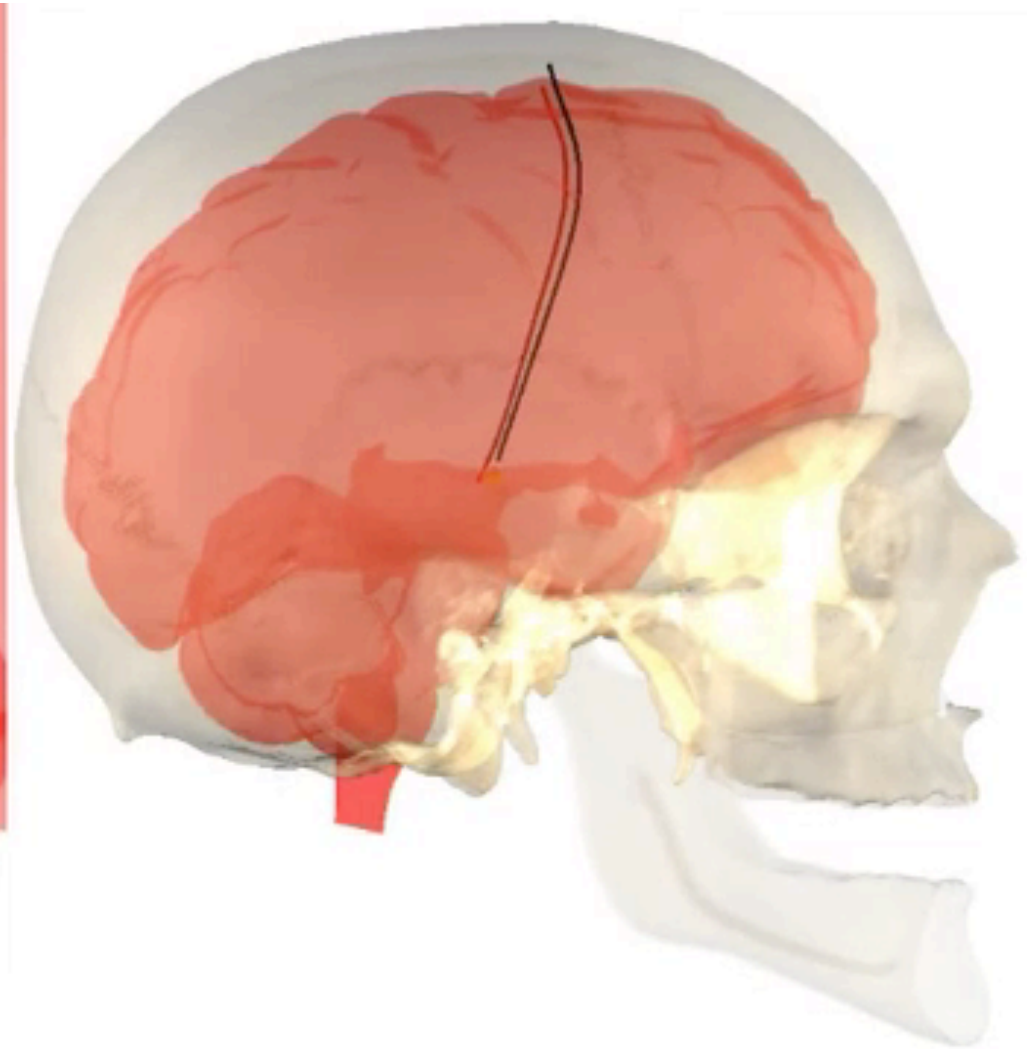
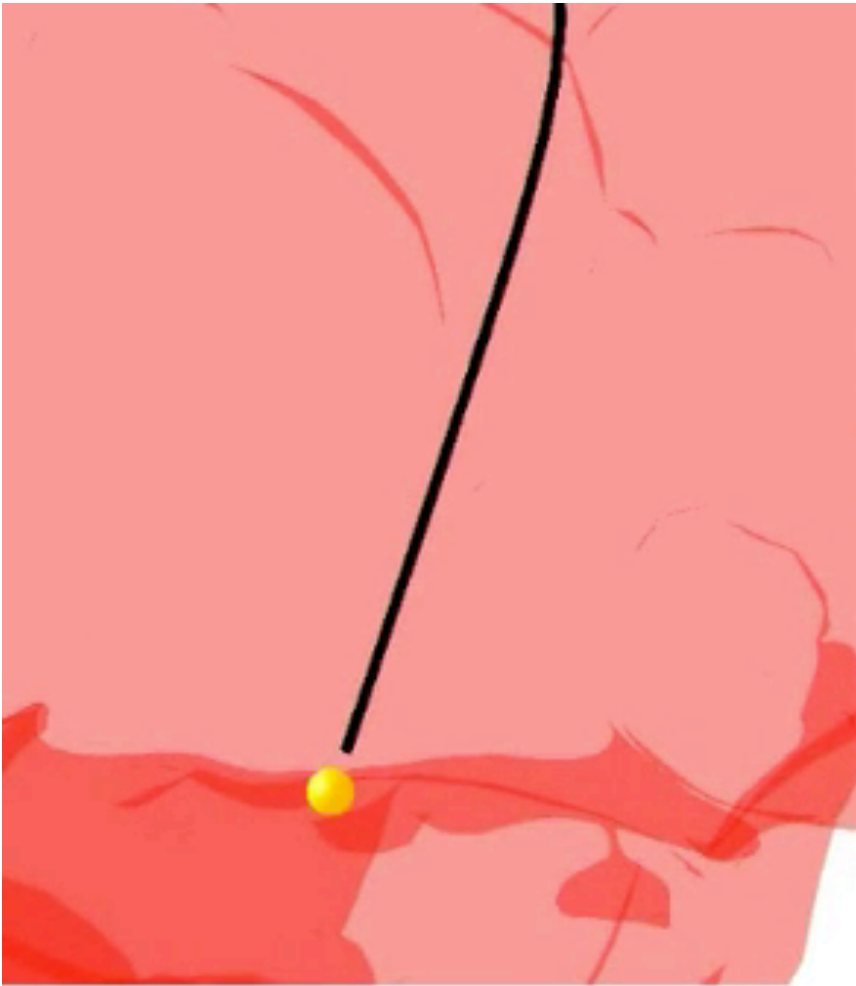
**A
POSTERIORI
ERROR**

Validation & parameter identification

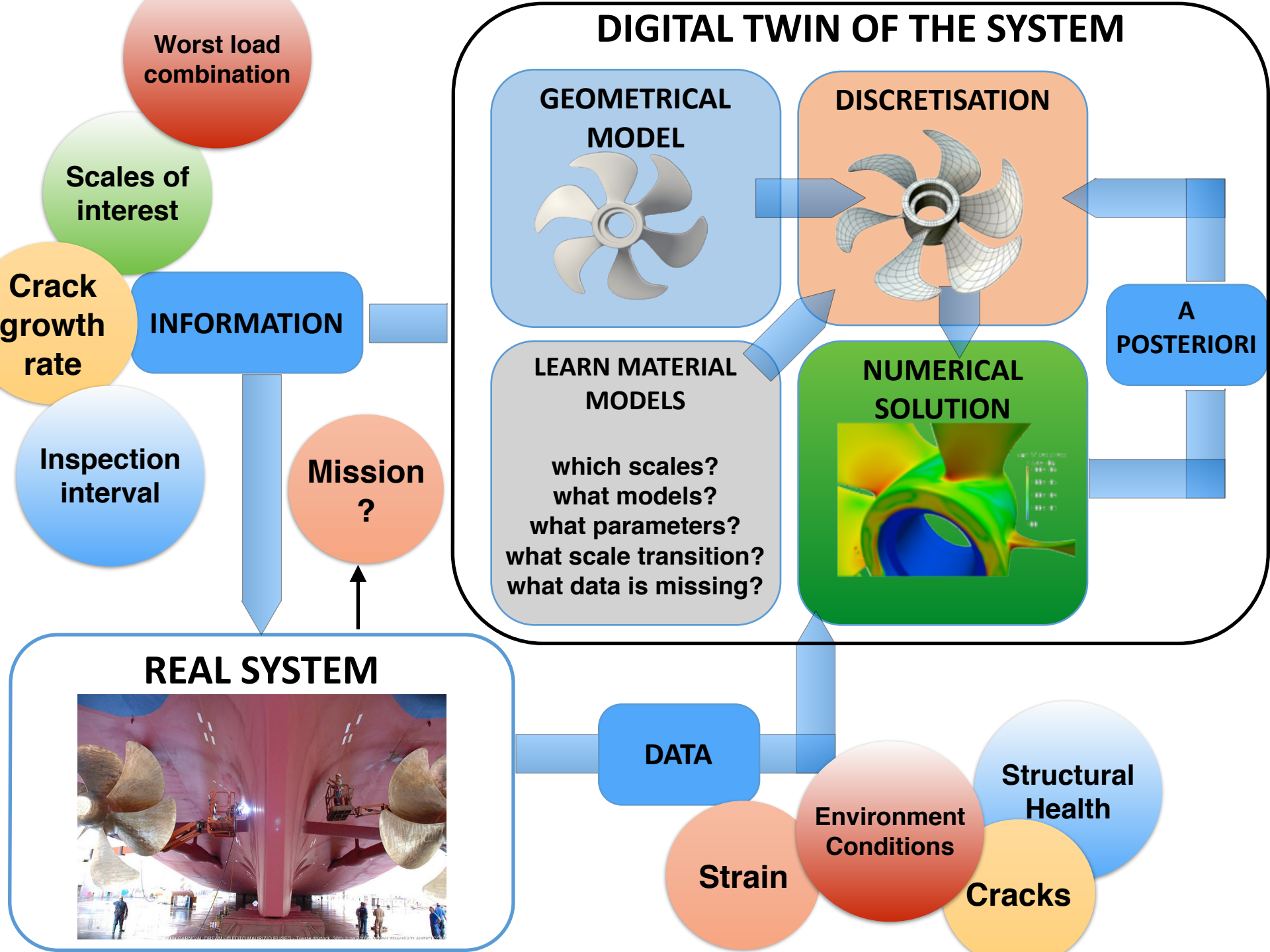
EXPERIMENTS

CONVENTIONAL APPROACH

When the material model is not known, this conventional approach is inadequate



Deep-brain stimulation



Discretization

- ➔ partition of unity enrichment
- ✓ (enriched) meshless methods
- ✓ level sets

- ➔ isogeometric analysis
- ➔ implicit boundaries

Model reduction

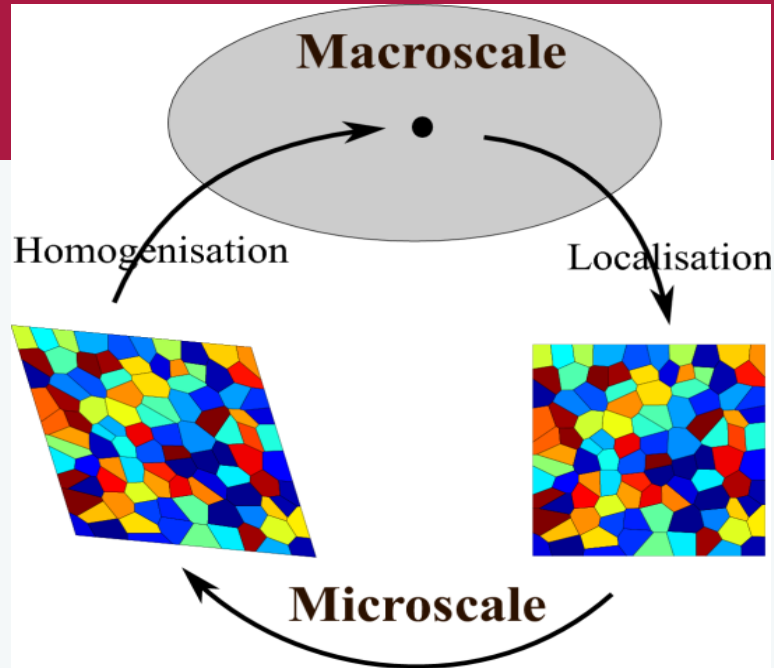
- ✓ multi-scale & homogenisation
- ✓ algebraic model reduction (using POD)
- ✓ Newton-Krylov, “local/global”, domain decomposition

Error control

- ✓ XFEM: goal-oriented error estimates
 - ▶ used by CENAERO (Morfeo XFEM)
- ✓ meshless methods for fracture
- ✓ error estimation for reduced models

- Homogenisation (FE², etc.) - Hierarchical
- Concurrent and hybrid (bridging domain, ARLEQUIN, etc.)
- Enrichment (PUFEM, XFEM, GFEM)
- Model reduction (algebraic)

Reduction methods based on homogenisation



Definition of an RVE

$$l^c \gg l^f \gg l^g$$

Coupling of macroscopic and microscopic levels

The volume averaging theorem is postulated for:

1) Strain tensor:

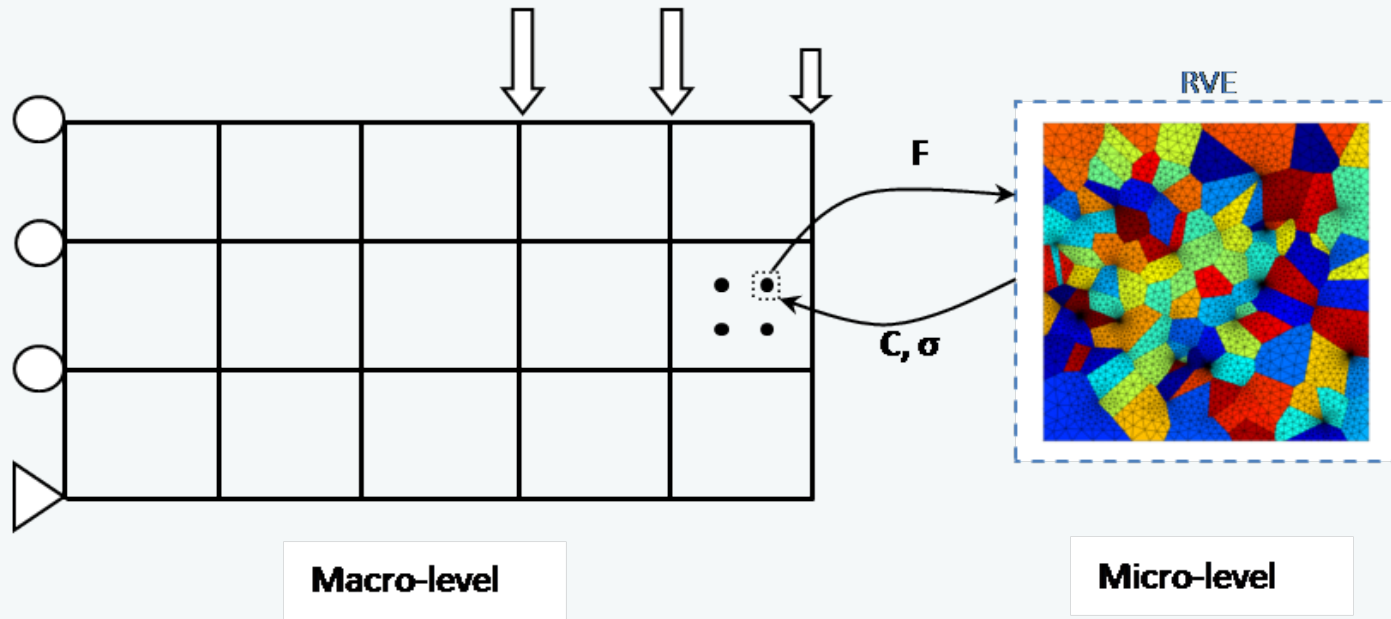
2) Virtual work (Hill-Mandel condition):

3) Stress tensor:

$$\epsilon^c = \frac{1}{|\Omega(\mathbf{x}^c)|} \int_{\partial\Omega(\mathbf{x}^c)} \mathbf{u}^f \otimes_s \mathbf{n} \, d\Gamma$$

$$\sigma^c : \delta\epsilon^c = \frac{1}{|\Omega(\mathbf{x}^c)|} \int_{\partial\Omega(\mathbf{x}^c)} \mathbf{t}^f \cdot \delta\mathbf{u}^f \, d\Gamma$$

$$\sigma^c = \frac{1}{|\Omega(\mathbf{x}^c)|} \int_{\partial\Omega(\mathbf{x}^c)} \mathbf{t}^f \otimes \mathbf{x}^f \, d\Gamma$$

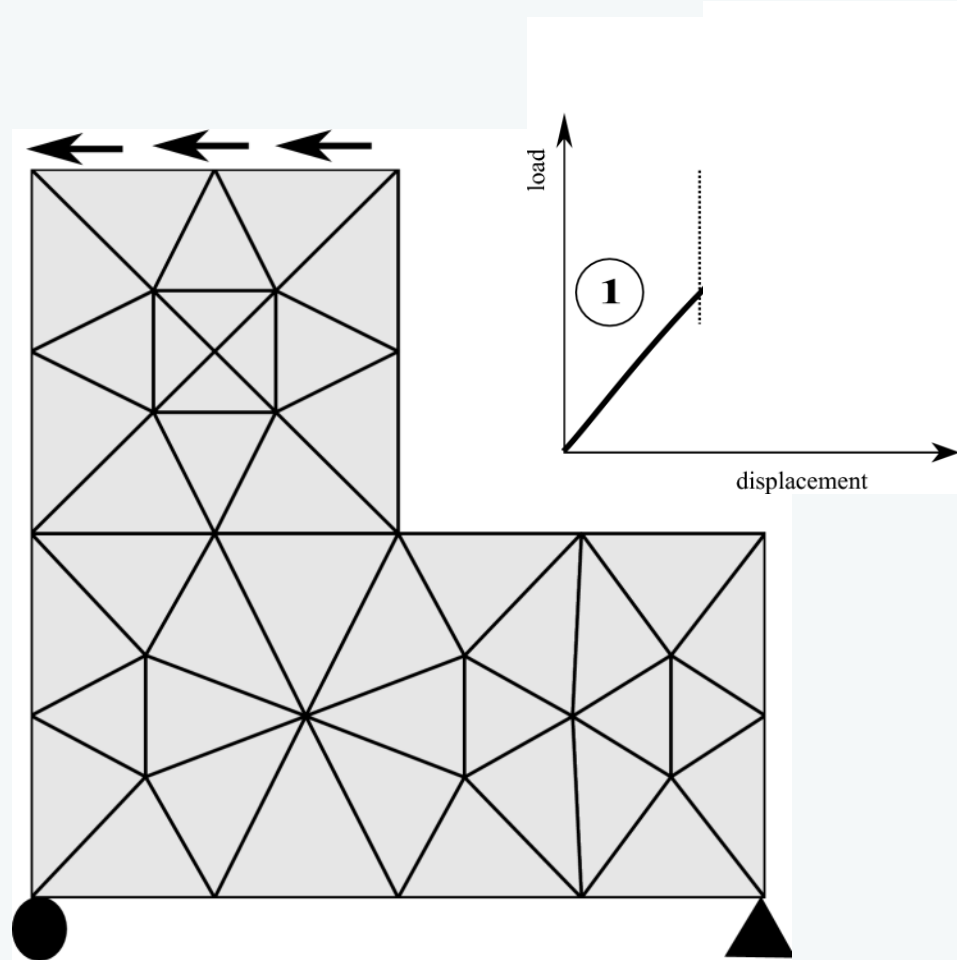


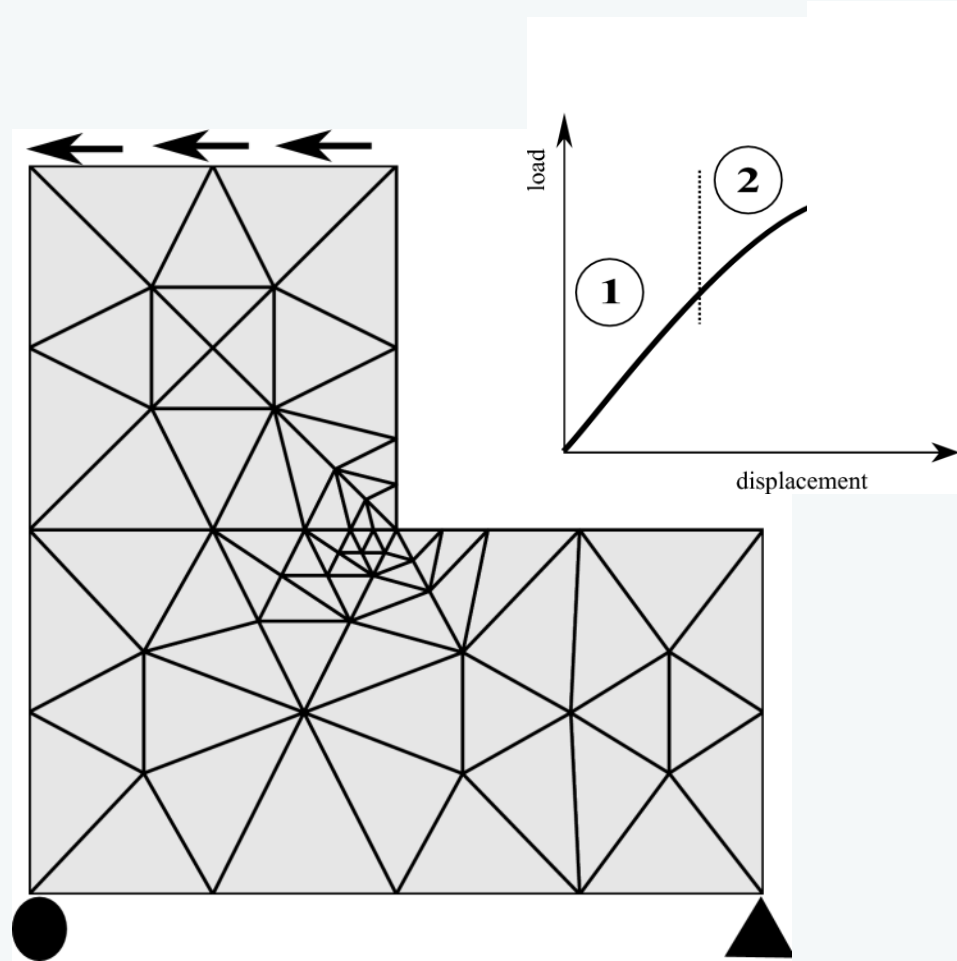
Advantages and abilities:

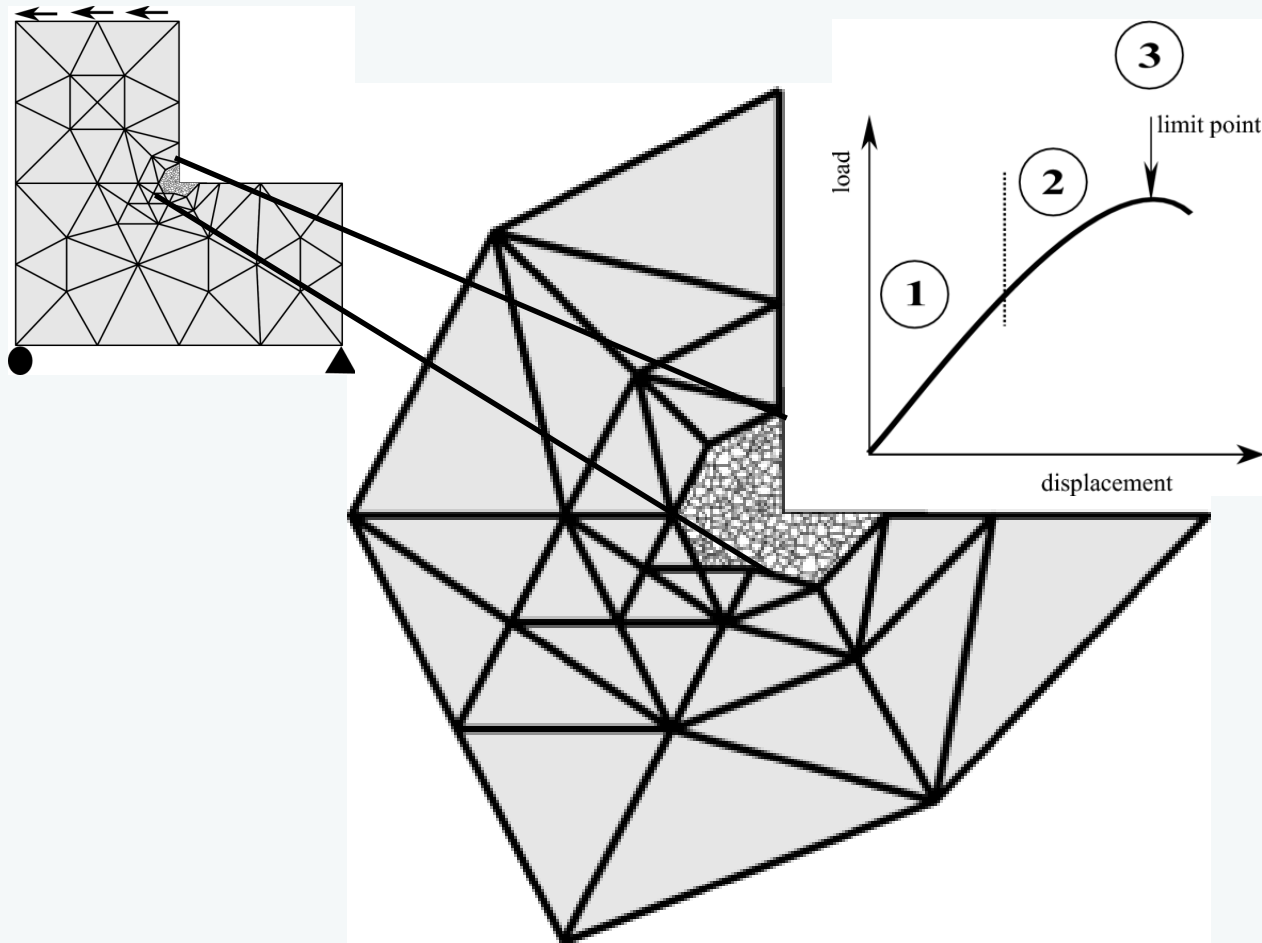
- The macroscopic constitutive law is not required
- Non-linear material behaviour can be simulated
- Microscale behaviour of material is monitored at each load step

Drawbacks:

- In softening regime:
- Lack of scale separation
 - Macroscale mesh dependence

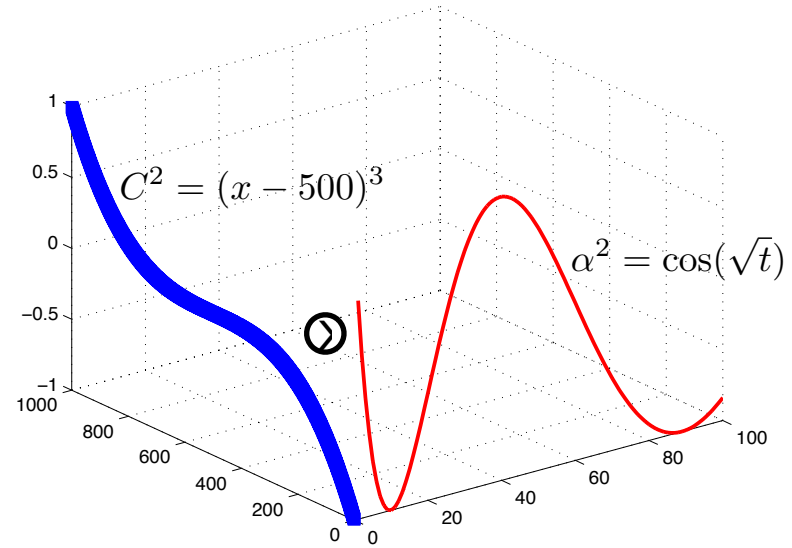
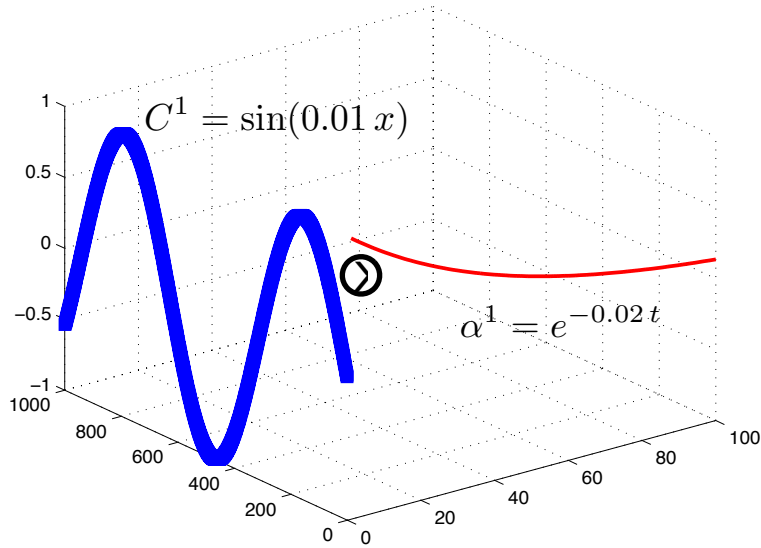


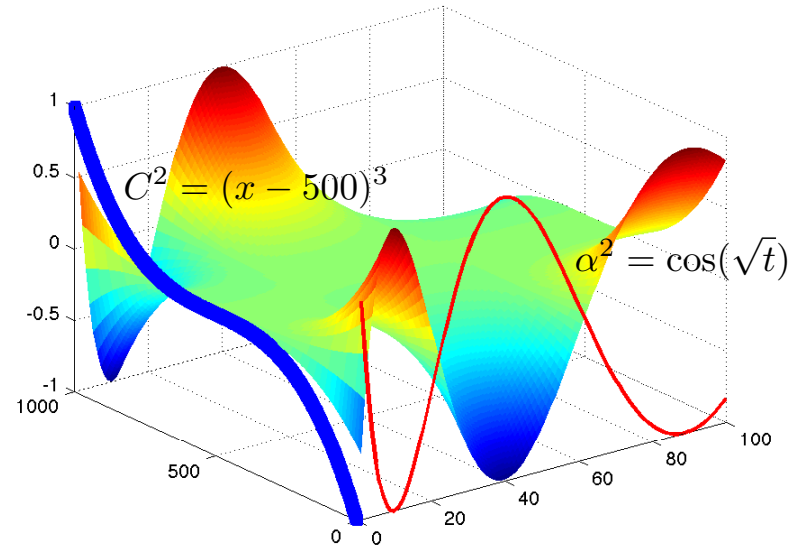
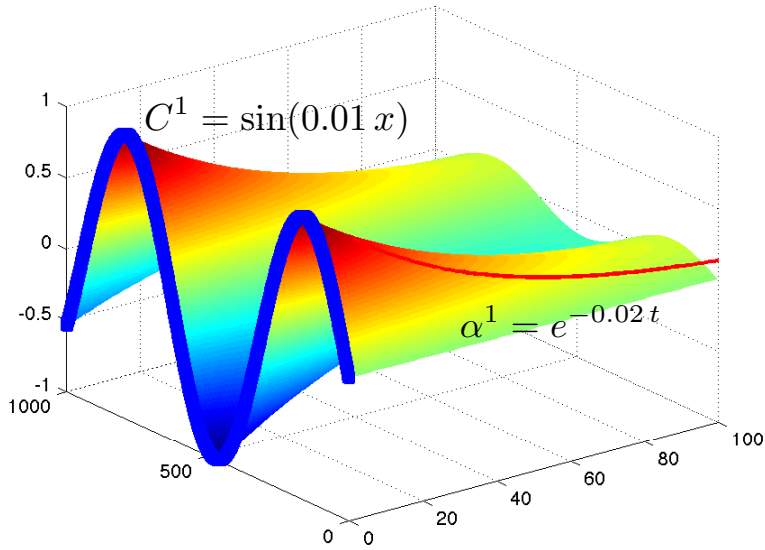


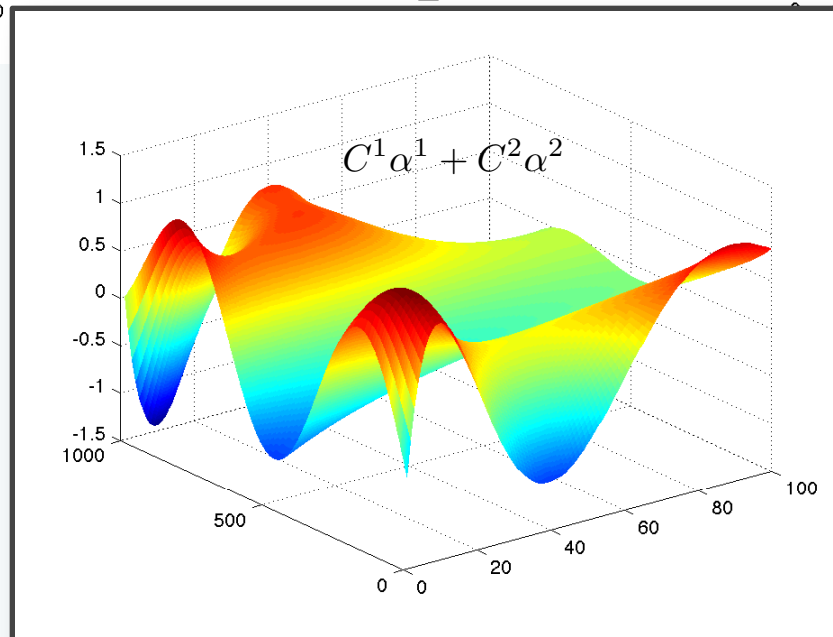
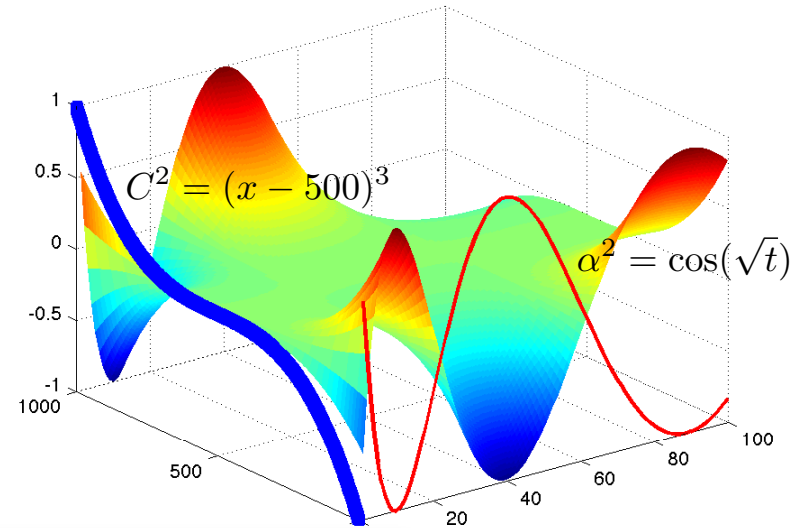
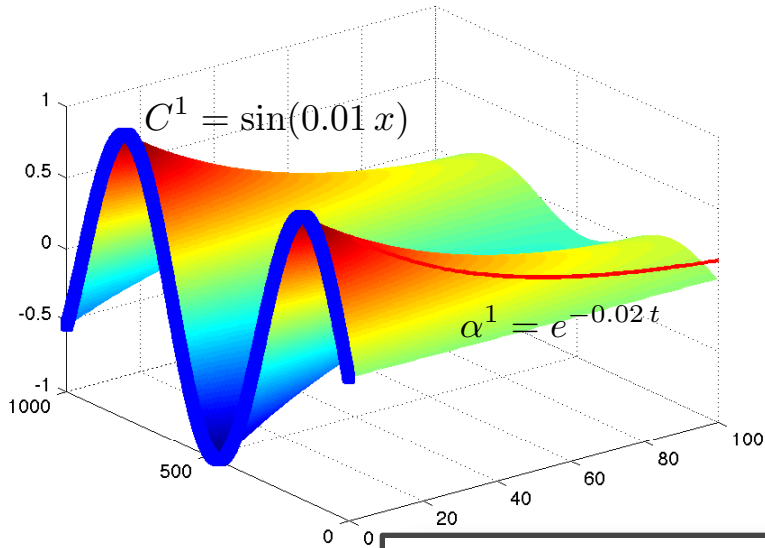


Details in Phil. Magazine, 2015, Akbari, Kerfriden, Bordas

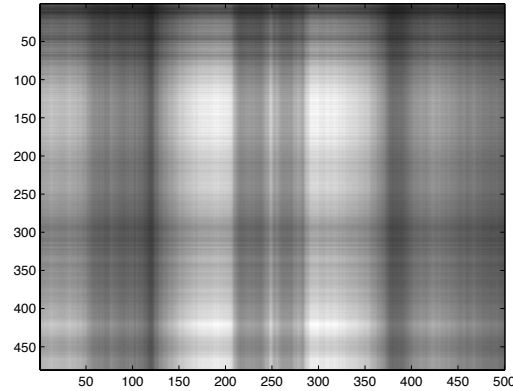
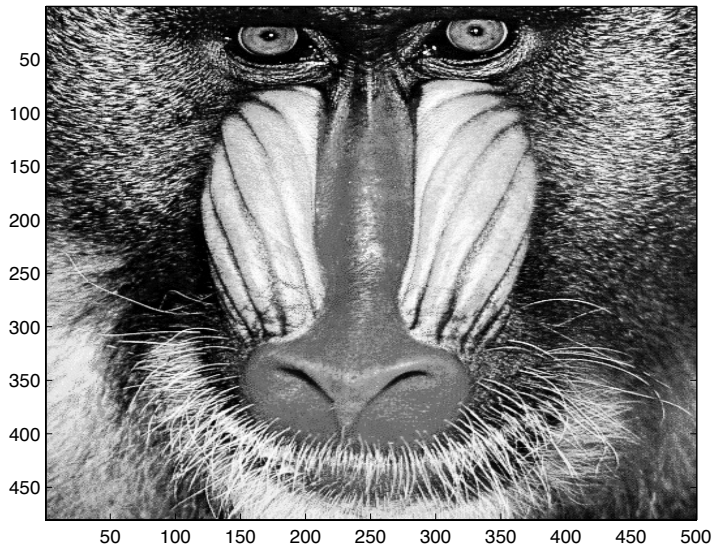
Reduction methods based on algebraic reduction







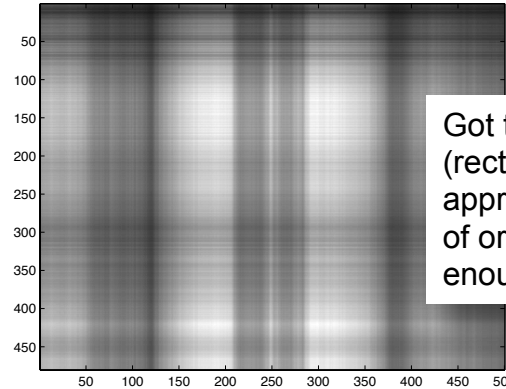
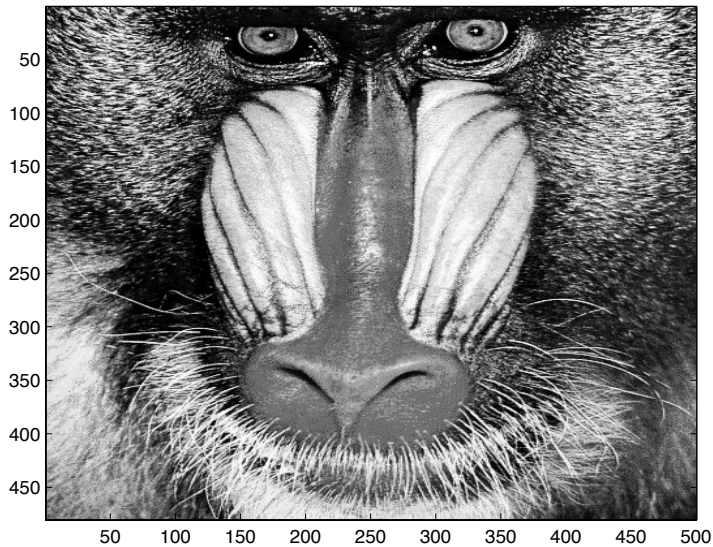
Very rich approximations!



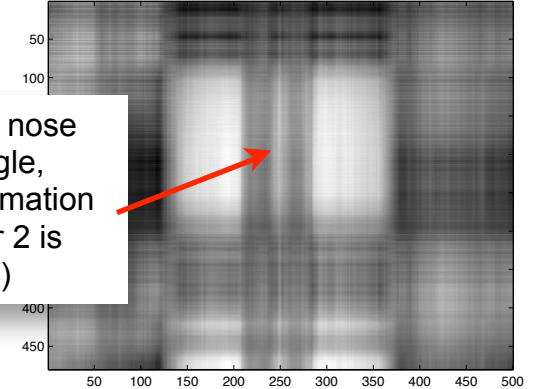
$n_c = 1$

$$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} C_x^i(x_i) C_y^i(y_i)$$

$$(C_x^i, C_y^i)_{i \in \llbracket 1, n_c \rrbracket} = \operatorname{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$$



$n_c = 1$

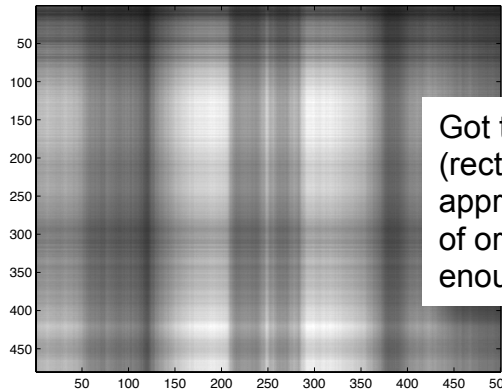
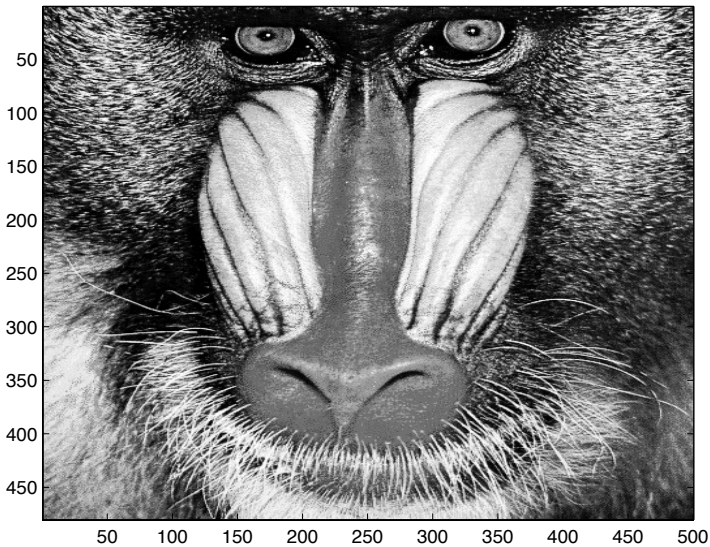


$n_c = 2$

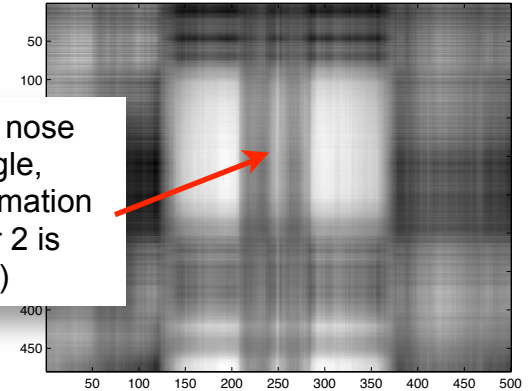
Got the nose
(rectangle,
approximation
of order 2 is
enough)

$$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} \underline{C}_x^i(x_i) \underline{C}_y^i(y_i)$$

$$(C_x^i, C_y^i)_{i \in \llbracket 1, n_c \rrbracket} = \operatorname{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$$

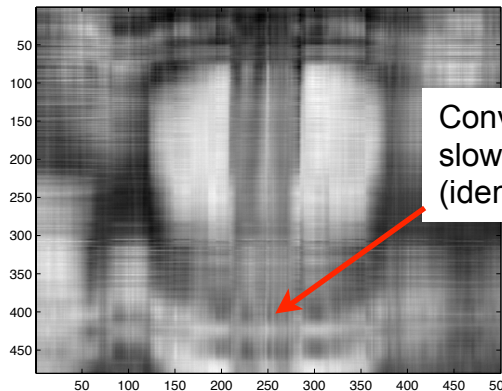


$n_c = 1$

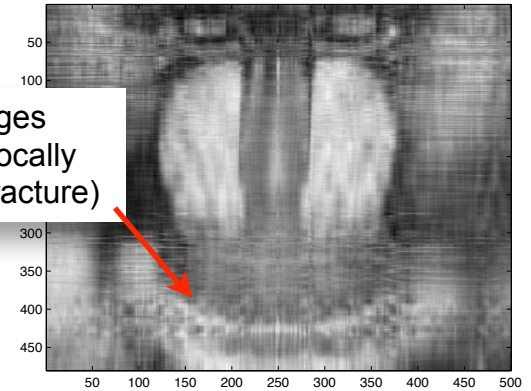


Got the nose (rectangle, approximation of order 2 is enough)

$n_c = 2$

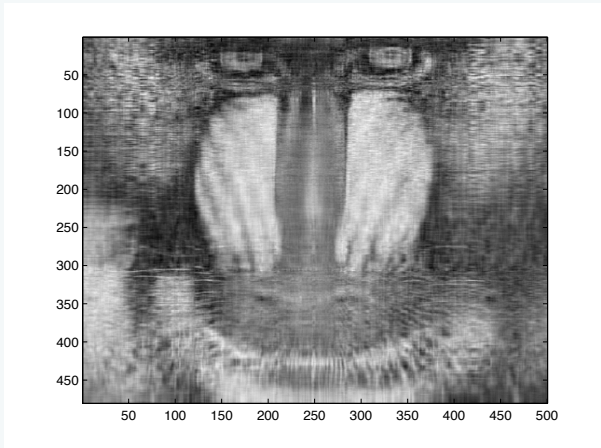


$n_c = 5$



Converges slowly locally (idem fracture)

$n_c = 10$



$n_c = 20$

$$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} \underline{C}_x^i(x_i) \underline{C}_y^i(y_i)$$

$$(C_x^i, C_y^i)_{i \in [1, n_c]} = \operatorname{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$$

- Search for the solution in space / time / parameter in a product space:

$$\bar{\mathbf{U}} : \mathcal{U}_{\text{sep}} = \mathbb{R}^n \times \mathcal{T} \times \mathcal{P} \rightarrow \mathbb{R}^n$$

$$\bar{\mathbf{U}}(t, \mu) = \sum_{i=1}^{n_C} \underline{\mathbf{C}}_i \beta_i(t) \gamma_i(\mu),$$

$$\underline{\mathbf{C}}^i \in \mathbb{R}^n$$

$$\beta^i : \mathcal{T} \rightarrow \mathbb{R}, \quad \forall i \in \llbracket 1, n_C \rrbracket,$$

$$\gamma^i : \mathcal{P} \rightarrow \mathbb{R}, \quad \forall i \in \llbracket 1, n_C \rrbracket,$$

- Optimality of an expansion of order n_C with respect to a particular metric defined on \mathcal{U}_{sep}
 - ➡ different metrics lead to different methods, which have their pro/cons
 - ➡ Choice strongly dependent on the context
- ▶ Data compression: **POD** (Proper Orthogonal Decomposition) is a classical choice in dimension 2
- ▶ Data compression in many dimensions: **multilinear POD**
- ▶ Solver in many dimensions without *a priori* knowledge of the solution: **PGD**
- ▶ Model order reduction: **Snapshot POD, Snapshot PGD**
- ▶ Initialiser, preconditioners: **low-order POD, low-order PGD, Snapshot POD**

- One writes the classical POD problem:

find an orthonormal basis $\underline{\underline{\mathbf{C}}} \in \mathbb{R}^{n \times n_c}$, $\underline{\underline{\mathbf{C}}}^T \underline{\underline{\mathbf{C}}} = \underline{\underline{\mathbf{I}}}_d$ minimising the POD functional:

$$J_{\text{POD}}(\underline{\underline{\mathbf{C}}}) = \int_{t \in \mathcal{T}} \|\underline{\underline{\mathbf{U}}}(t) - \underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{C}}}^T \underline{\underline{\mathbf{U}}}(t)\|_2^2 dt$$

- Equivalently, look for a maximum of $\bar{J}_{\text{POD}}(\underline{\underline{\mathbf{C}}}) = \int_{t \in \mathcal{T}} \underline{\underline{\mathbf{U}}}(t)^T \underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{C}}}^T \underline{\underline{\mathbf{U}}}(t) dt = \text{Tr}(\underline{\underline{\mathbf{C}}}^T \underline{\underline{\mathbf{K}}} \underline{\underline{\mathbf{C}}})$

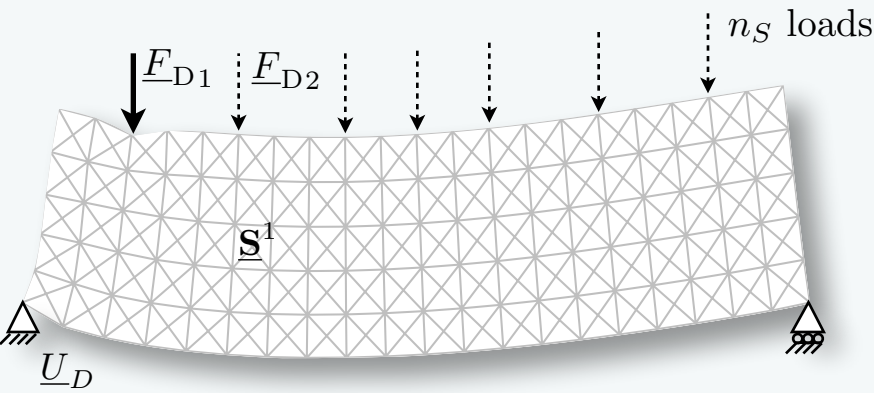
▶ Correlation operator: $\underline{\underline{\mathbf{K}}} = \int_{t \in \mathcal{T}} \underline{\underline{\mathbf{U}}}(t) \underline{\underline{\mathbf{U}}}(t) dt$

- Solution: eigenvalue problem $\underline{\underline{\mathbf{K}}} \underline{\underline{\phi}}^k = \lambda^k \underline{\underline{\phi}}^k$ where $(\lambda^k)_{k \in \llbracket 0, n \rrbracket}$ in decreasing order

→ $\underline{\underline{\mathbf{C}}} = (\underline{\underline{\phi}}^1 \quad \underline{\underline{\phi}}^2 \quad \dots \quad \underline{\underline{\phi}}^{n_c})$

→ $\int_{t \in \mathcal{T}} \alpha^i \alpha^j dt = \delta_{ij} \lambda^i$

- Error $J_{\text{POD}}(\underline{\underline{\mathbf{C}}}) = \sum_{k=n_c+1}^n \lambda^k$



(1) Solve FINE for n_S parameters (EXPENSIVE!)

$$\underline{\underline{S}} = (\underline{S}^1 \quad \underline{S}^2 \quad \dots \quad \underline{S}^{n_S})$$

(2) Singular value decomposition

$$\underline{\underline{S}} = \underline{\underline{U}} \underline{\underline{\Sigma}} \underline{\underline{V}}^T = \sum_{k=1}^{n_S} \Sigma^k \underline{U}^k \underline{V}^{kT}$$

n_S solutions, sorted by relevance

where $(\Sigma^k)_{k \in [1 \ n_S]}$ in decreasing order

(3) Truncation

Initial set of equations

$$\underline{\underline{F}}_{\text{Int}} (\underline{\underline{U}}) + \underline{\underline{F}}_{\text{Ext}} = 0$$

(4) Galerkin orthogonality

$$\underline{\underline{C}}^T \underline{\underline{F}}_{\text{int}} (\underline{\underline{C}} \underline{\underline{\alpha}}) + \underline{\underline{C}}^T \underline{\underline{F}}_{\text{ext}} = 0$$

Approximation of the solution in a space of small dimension (n_c)

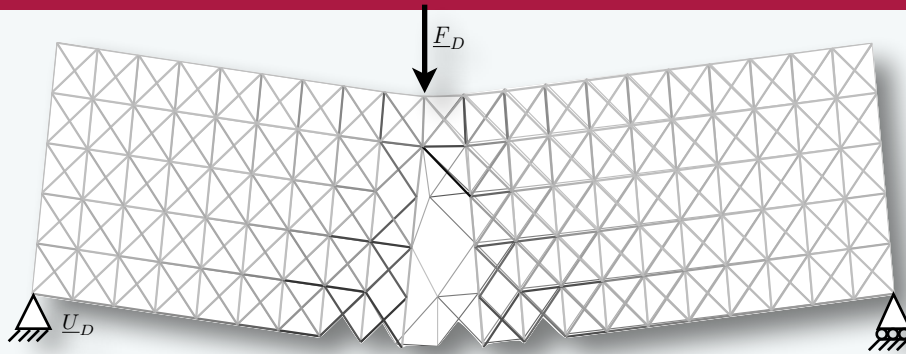
Family of representative solutions

$$\underline{\underline{U}} = \underline{\underline{C}} \underline{\underline{\alpha}}$$

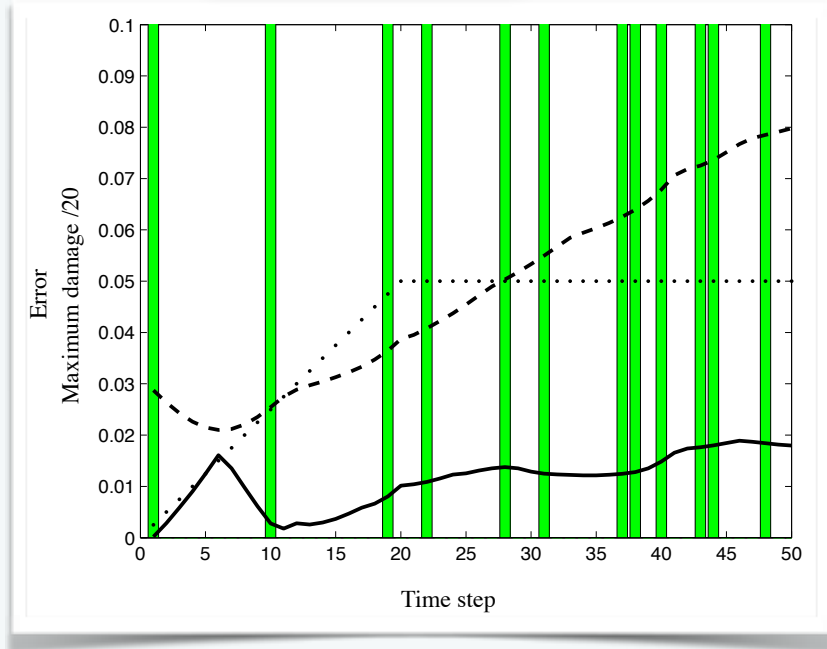
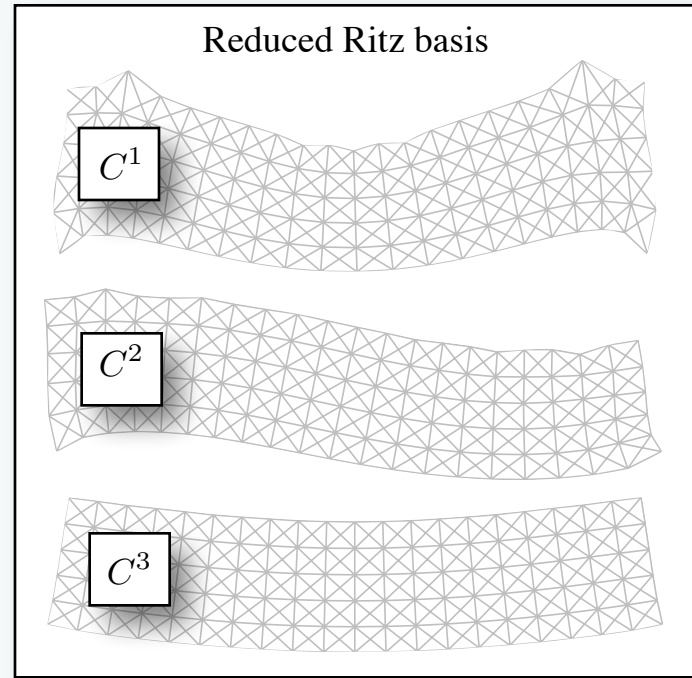
Solution Coefficients

Reduced basis: family of representative solutions

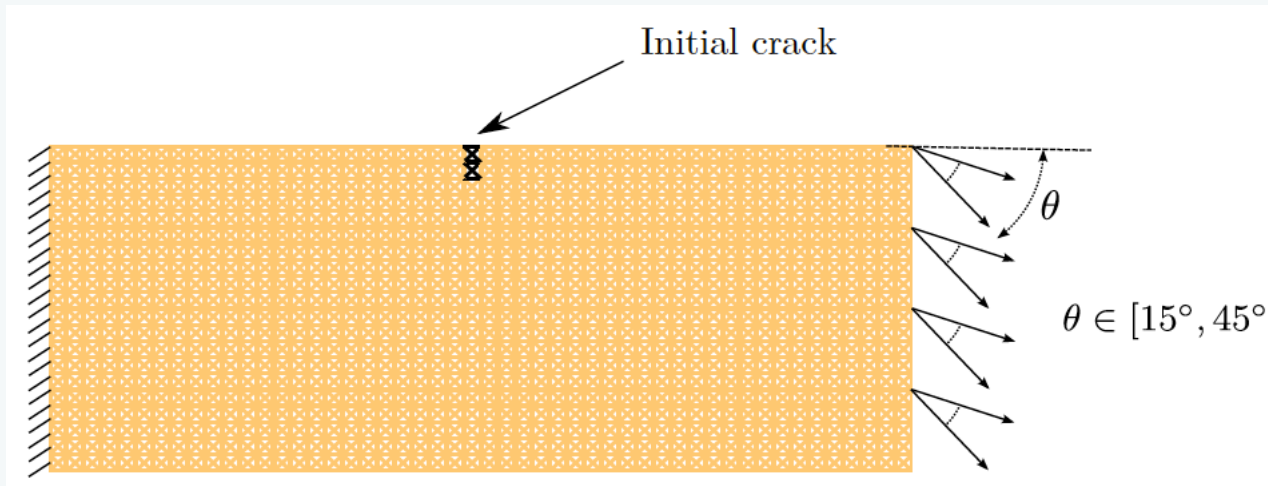
$\underline{\underline{C}} = (\underline{U}^1 \quad \underline{U}^2 \quad \dots \quad \underline{U}^{n_c})$

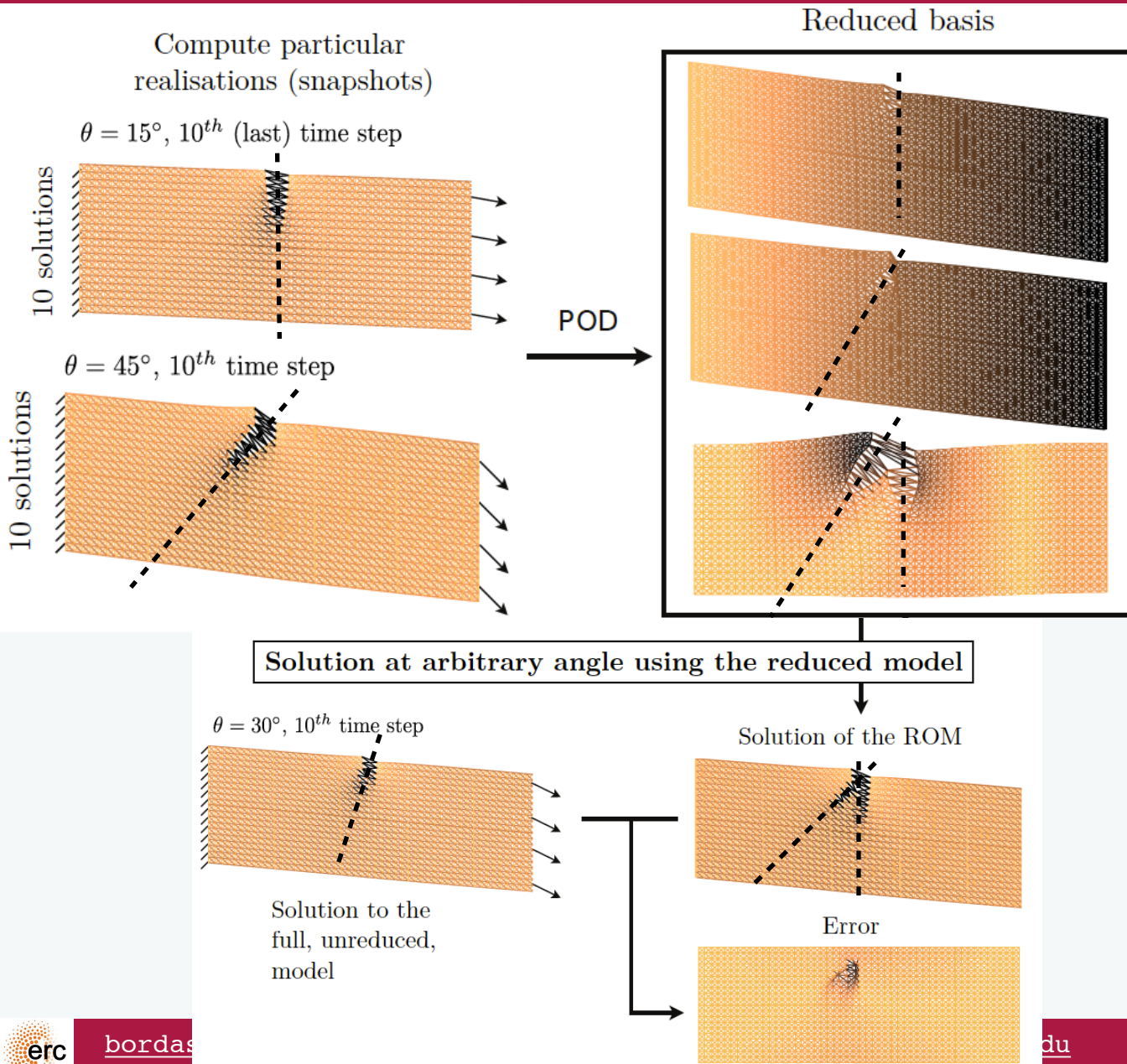


This solution is not in the snapshot !

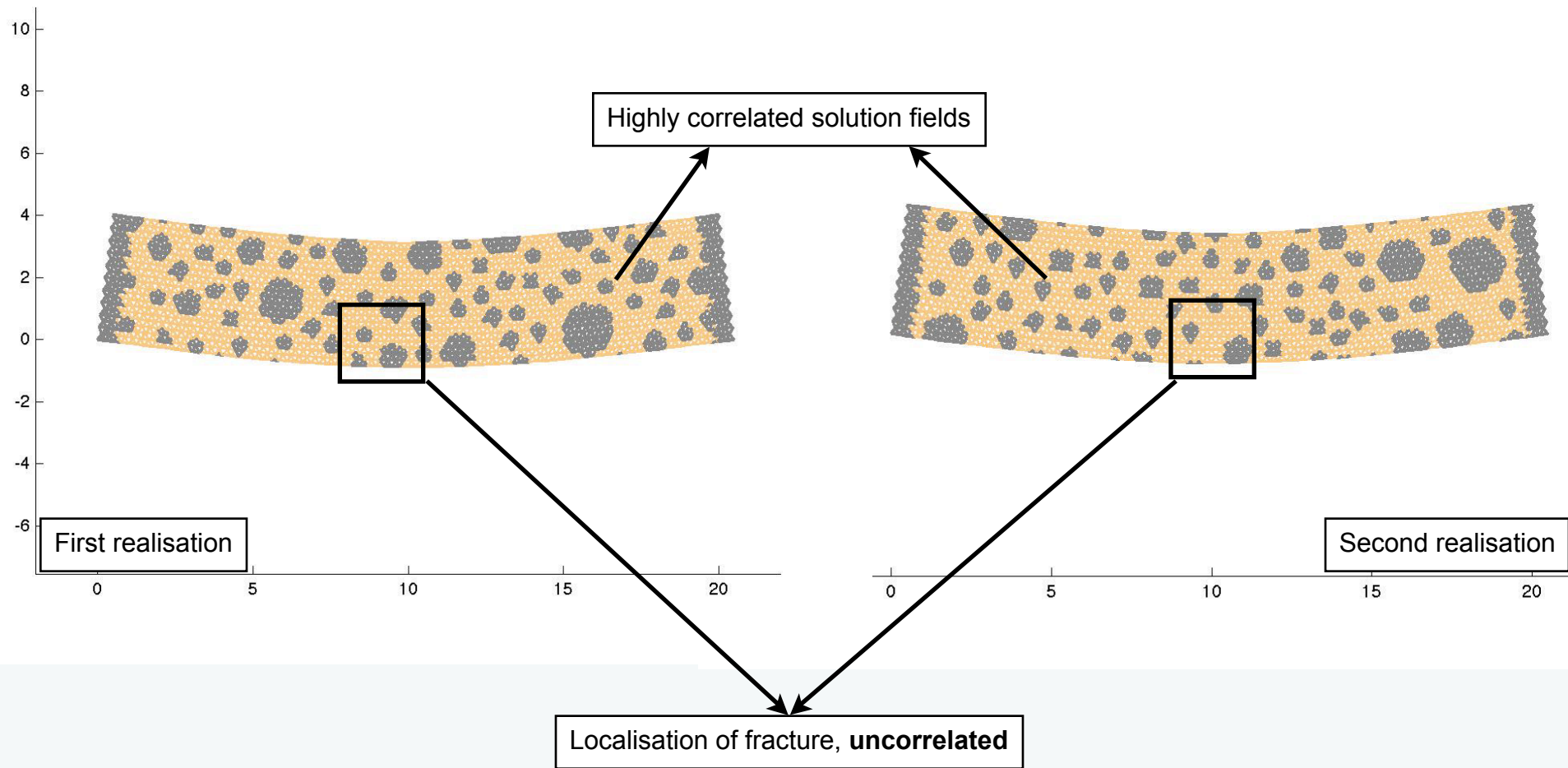


- P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. *Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems.* Computer Methods in Applied Mechanics and Engineering, 200(5-8): 850-866, 2011.





- ▶ The POD solution is not able to reproduce the solution in the cracked area
- ▶ Due to lack of correlation introduced by crack growth
- ▶ Leads to a local projection error

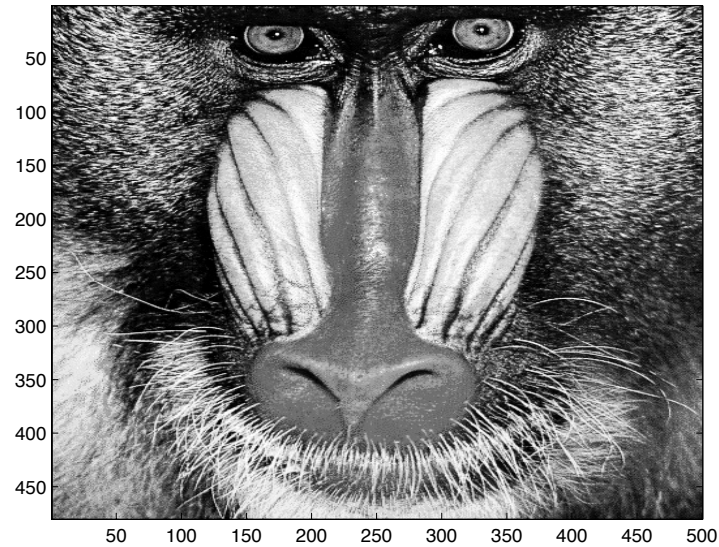


➔ Direct numerical simulation: efficient preconditioner?

➔ Reduced order modelling?

➔ Adaptive coupling?

THE RETURN OF THE MONKEY!



What can we do to address this lack of separation
of scales/reducibility?

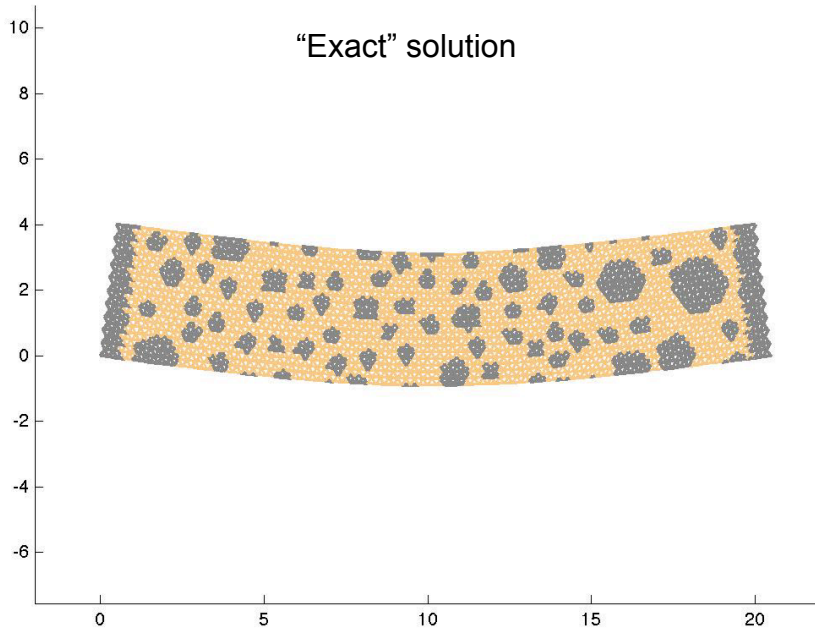
P. Kerfriden, P. Gosselet, S. Adhikari, and S. Bordas. Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: an adaptive model order reduction for highly nonlinear mechanical problems. *Computer Methods in Applied Mechanics and Engineering*, 200(5-8):850–866, 2011.

P. Kerfriden, J.C. Passieux, and S. Bordas. Local/global model order reduction strategy for the simulation of quasi-brittle fracture. *International Journal for Numerical Methods in Engineering*, 89(2):154–179, 2011.

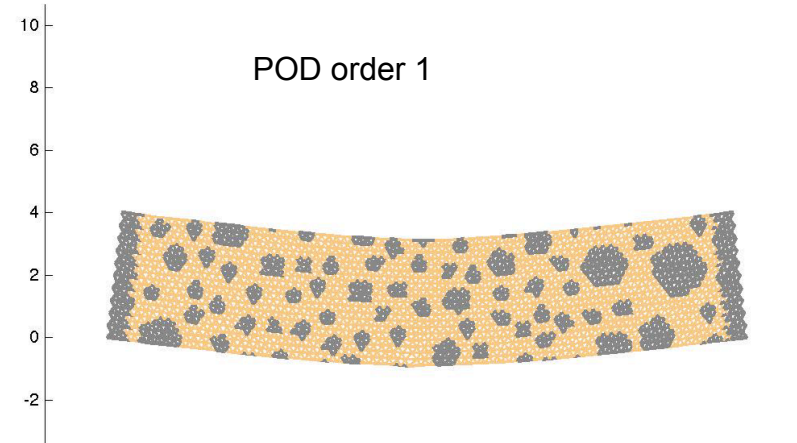
P. Kerfriden, K.M. Schmidt, T. Rabczuk, and Bordas S.P.A. Statistical extraction of process zones and representative subspaces in fracture of random composites. *Accepted for publication in International Journal for Multiscale Computational Engineering*, *arXiv:1203.2487v2*, 2012.

Snapshot POD (snapshot space is spanned by the ensemble of solutions at all time steps)

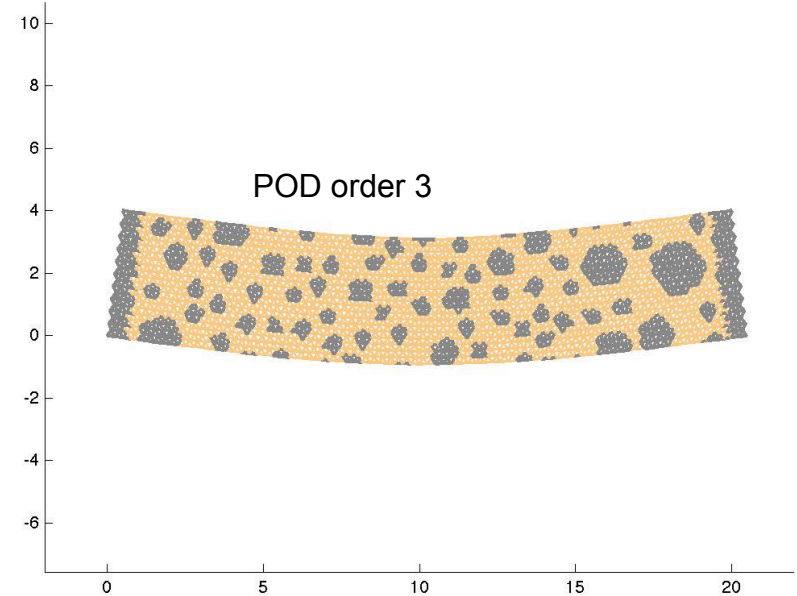
“Exact” solution

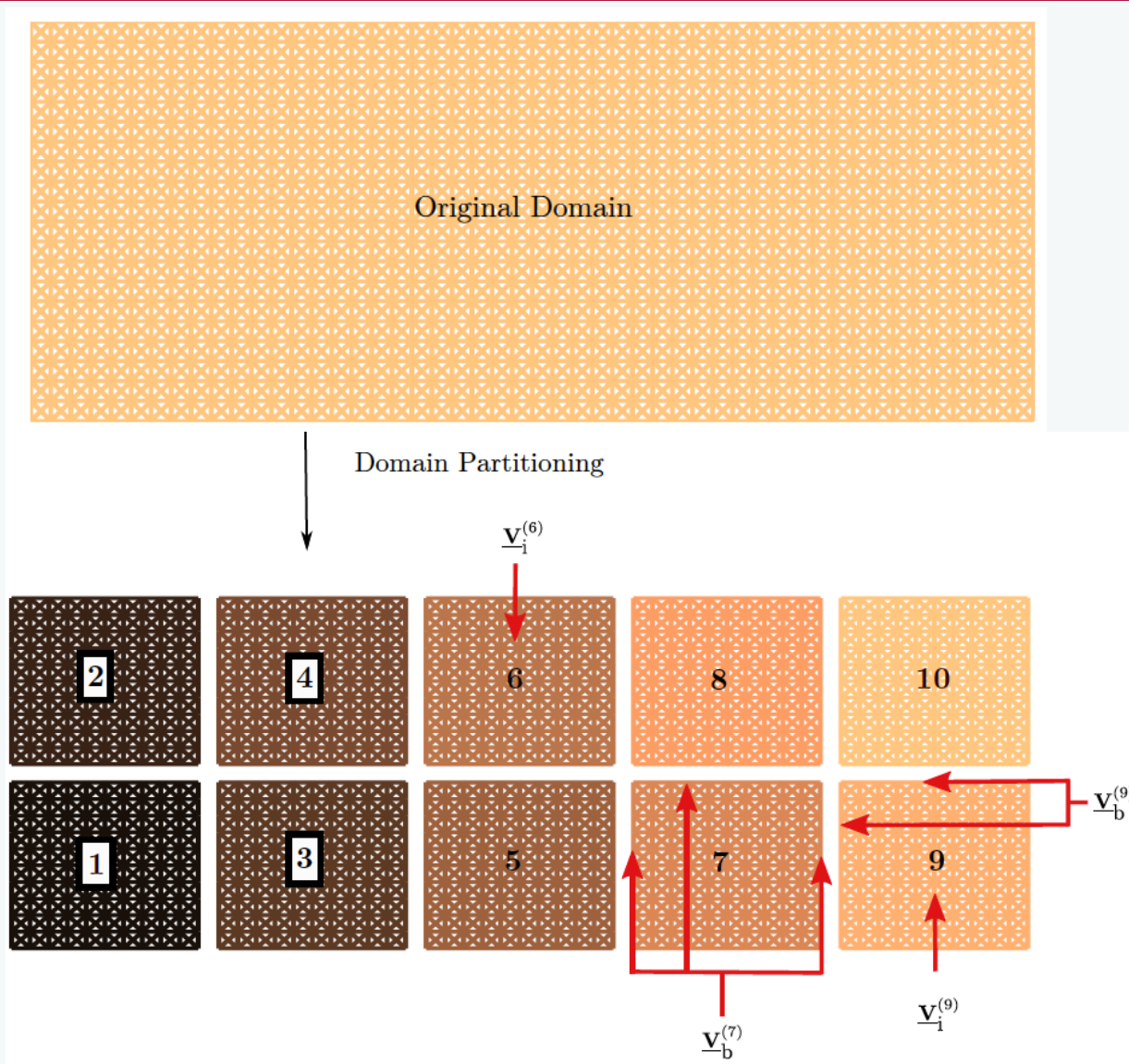


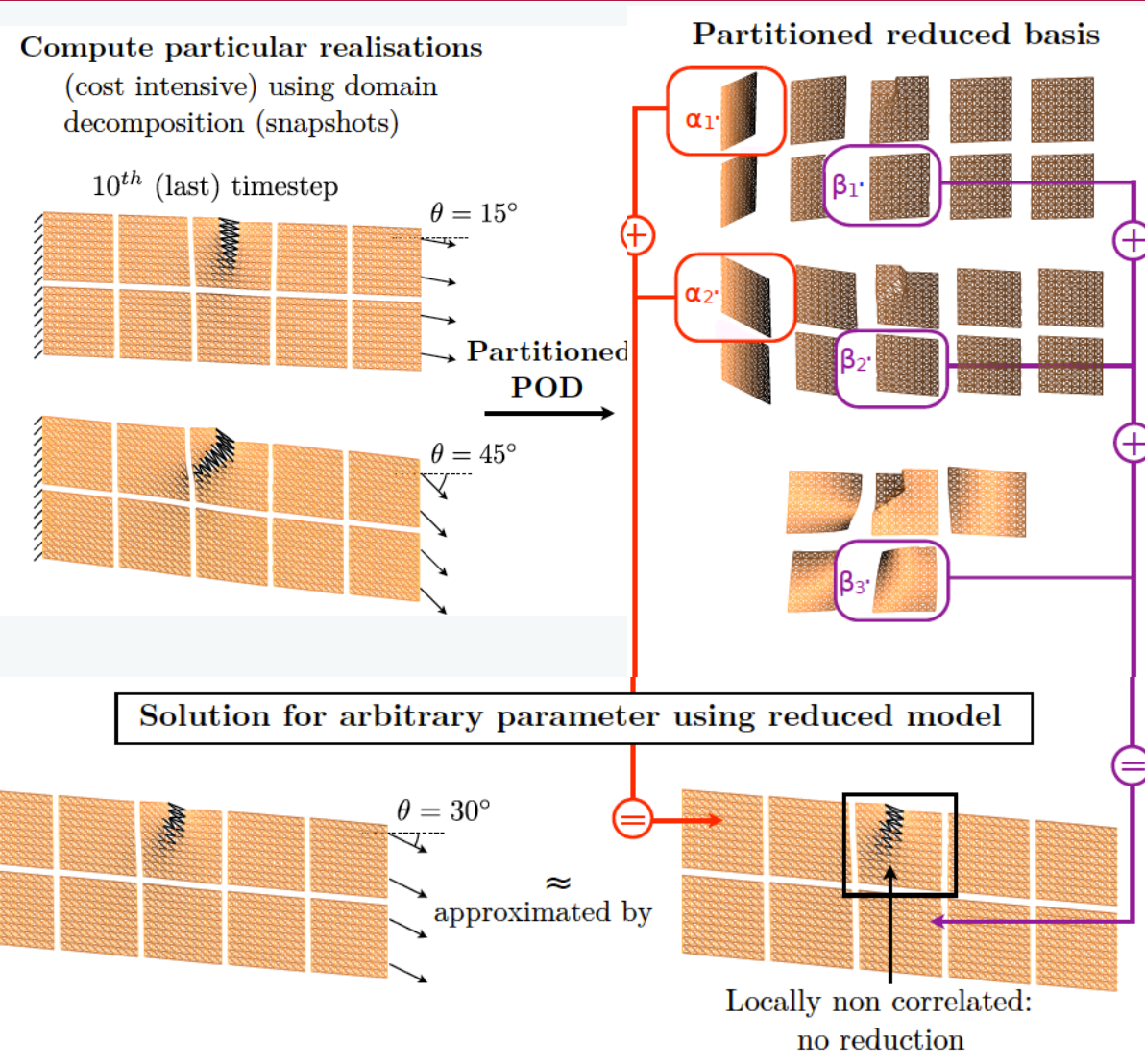
POD order 1



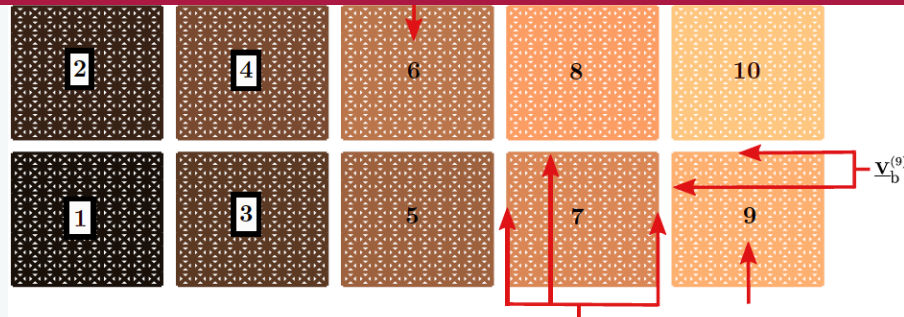
POD order 3



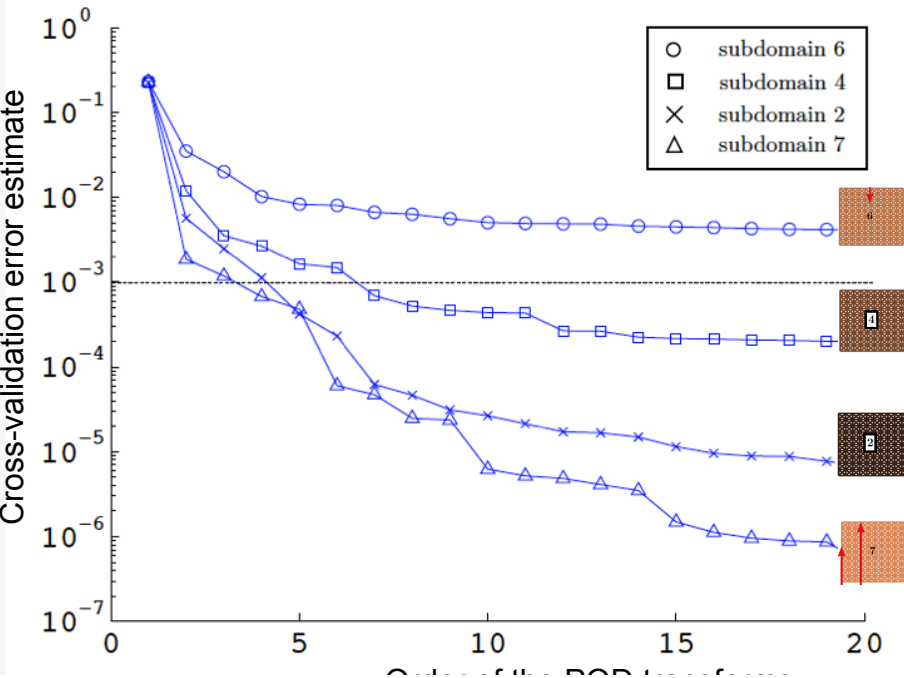




- ▶ Decompose the structure into subdomains
- ▶ Perform a reduction in the highly correlated region
- ▶ Couple the reduced to the non-reduced region by a primal Schur complement

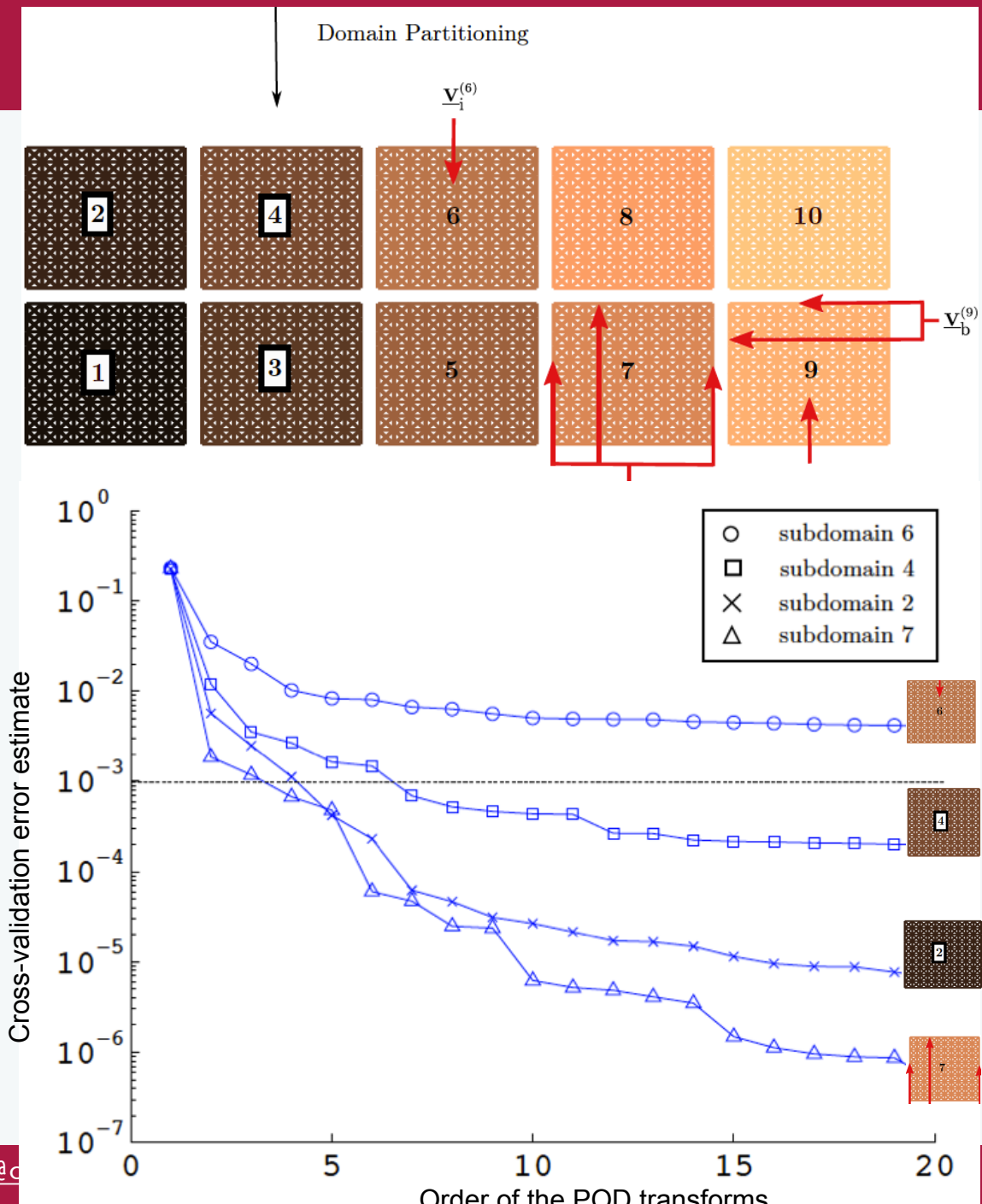


- Reduced subspaces are independent and we assume a snapshot is *a priori* available
 - ▶ (1) Dimension of the local space for each subdomain?
 - ▶ (2) Is a given subdomain is reducible?
- (1) and (2) will be treated by cross-validation (e.g. W. J. Krzanowski. Cross-validation in principal component analysis. *Biometrics*, 43(3):575-584, 1987.)
 - ▶ **Training set:** snapshot
 - ▶ **Validation set:** set of additional finescale solutions
 - ▶ Independent training/validation avoids overfitting
 - ▶ Cross validation **emulates independence**. Error calculated using the local reduced basis obtained by a snapshot POD transform of all the available snapshot solutions except the one corresponding to the value of the summation variable.



- **NOTE:** If the snapshot is not assumed *a priori* then
 - ▶ Assess whether the snapshot contains sufficient information, and generate additional, suitable, data if required
 - ▶ Most analysis (mostly by statisticians) assume the snapshot is known *a priori*. Recent review: Hervé Abdi and Lynne J. Williams. *Principal component analysis*. Wiley Interdisciplinary Reviews: Computational Statistics, 2(4):433{459, 2010.

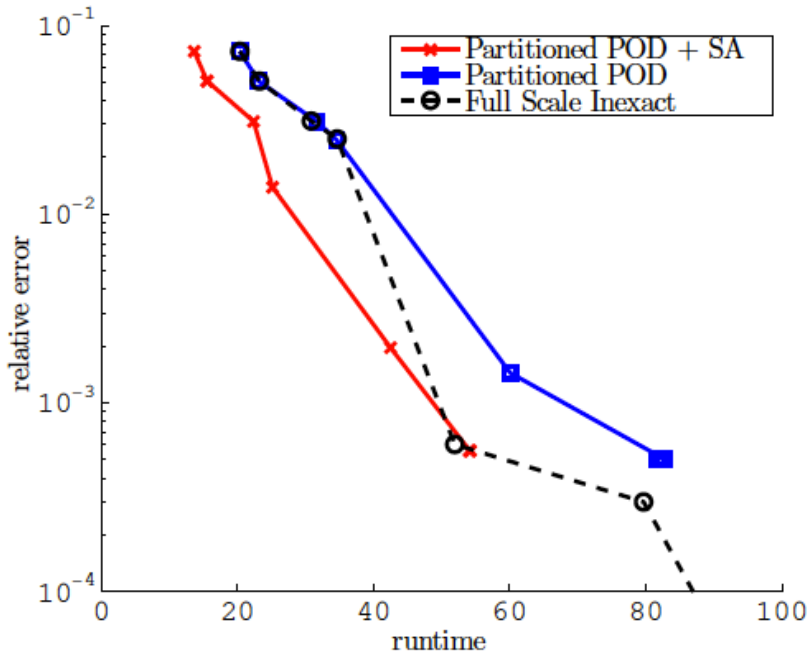
$$(\tilde{v}_{\text{snap}}^{(e)})^2 = \frac{\sum_{\mu \in \mathcal{P}^s} \sum_{t_n \in \mathcal{T}^h} \left\| \mathbf{U}_i(t_n, \mu) - \sum_{j=1}^{n_c^{(e)}} \left(\tilde{\mathbf{c}}_{i,j}^{(e),(\mu)T} \mathbf{U}_i(t_n, \mu) \right) \tilde{\mathbf{c}}_{i,j}^{(e),(\mu)} \right\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \sum_{\mu \in \mathcal{P}^s} \|\mathbf{U}_i(t_n, \mu)\|_2^2}$$



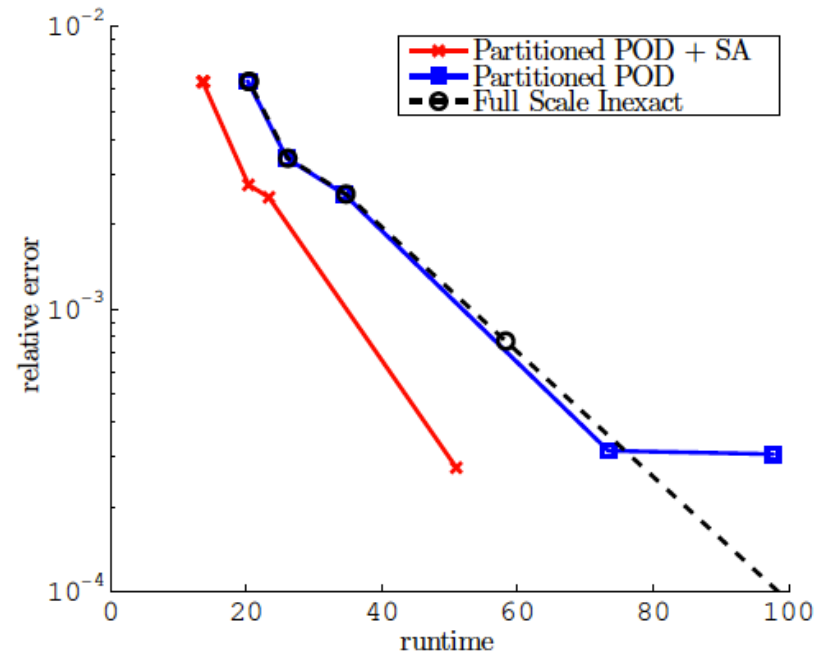
● Relative error

$$\nu^{\text{app},(\mu)}(\underline{\mathbf{U}}^{\text{app}})^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{app}}(t_n, \mu) - \underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}$$

40°



27°

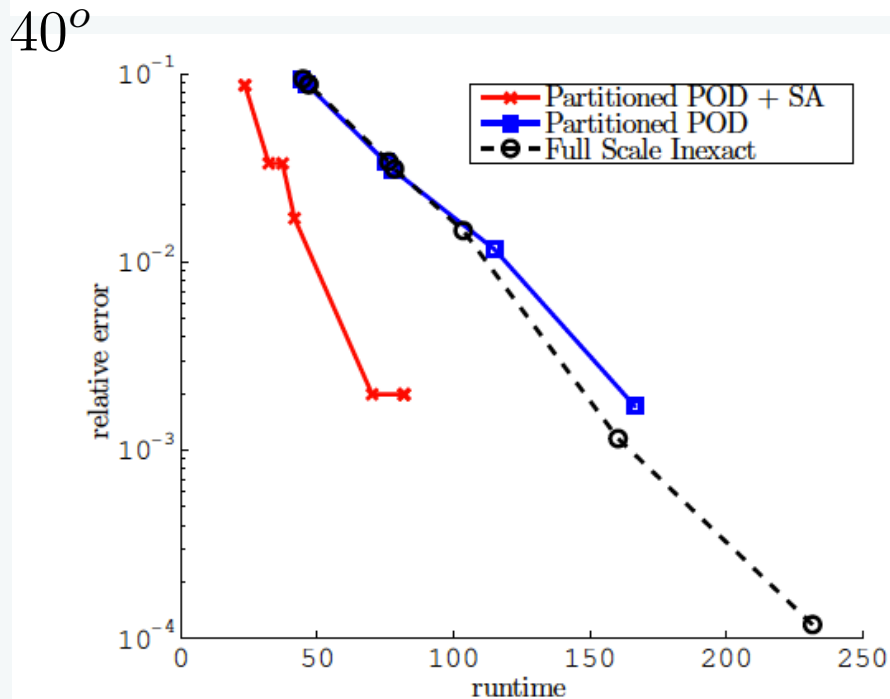


(a) Relative error for the different models using 121 nodes per subdomain

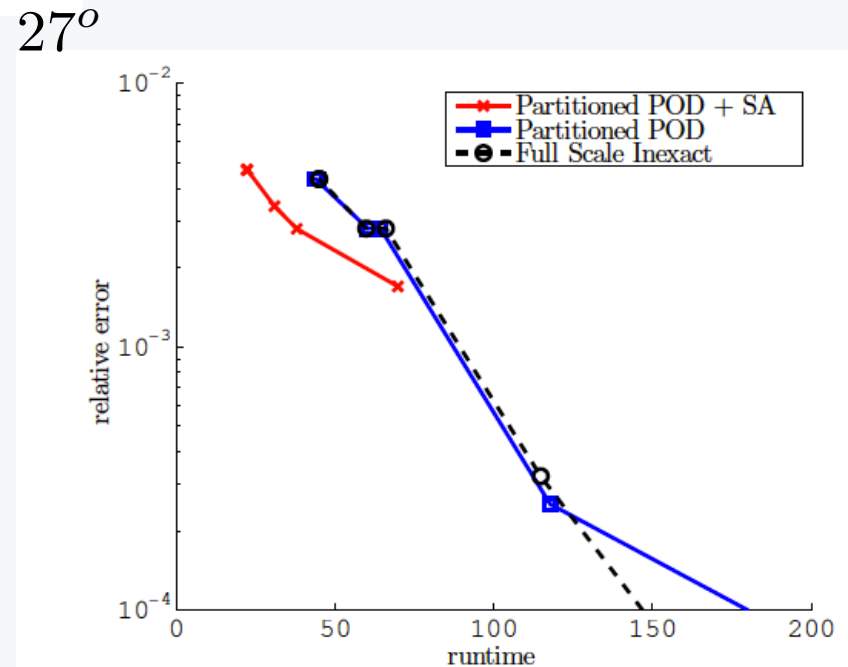
(a) Relative error for the different models using 121 nodes per subdomain

- Relative error

$$\nu^{\text{app},(\mu)}(\underline{\mathbf{U}}^{\text{app}})^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{app}}(t_n, \mu) - \underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}$$



(b) Relative error for the different models using 256 nodes per subdomain

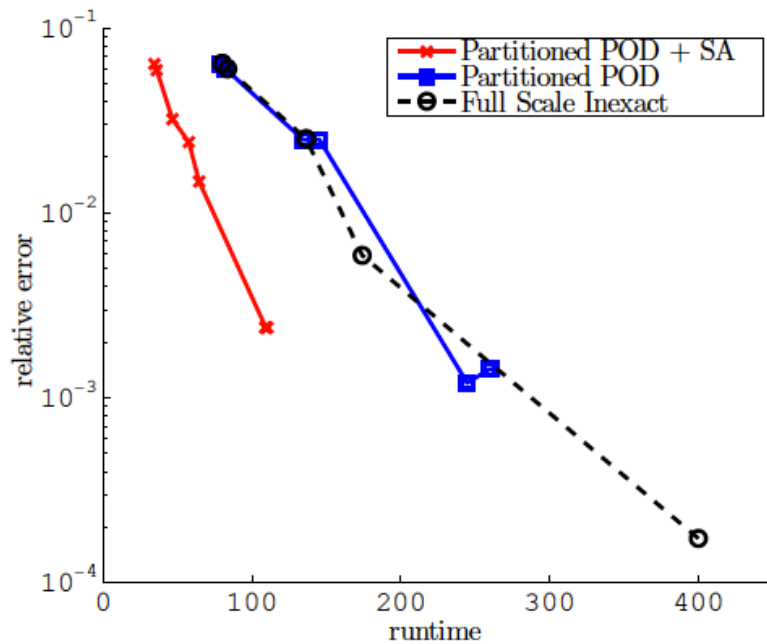


(b) Relative error for the different models using 256 nodes per subdomain

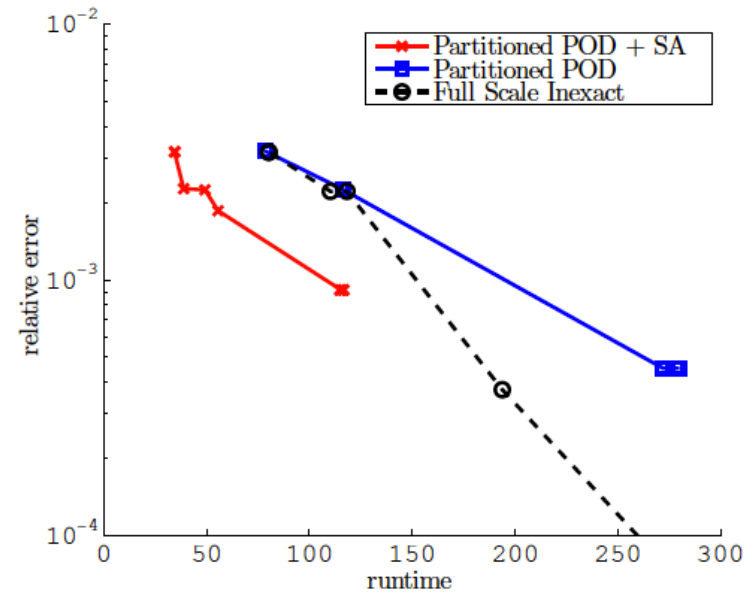
● Relative error

$$\nu^{\text{app},(\mu)}(\underline{\mathbf{U}}^{\text{app}})^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{app}}(t_n, \mu) - \underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}$$

40°



27°

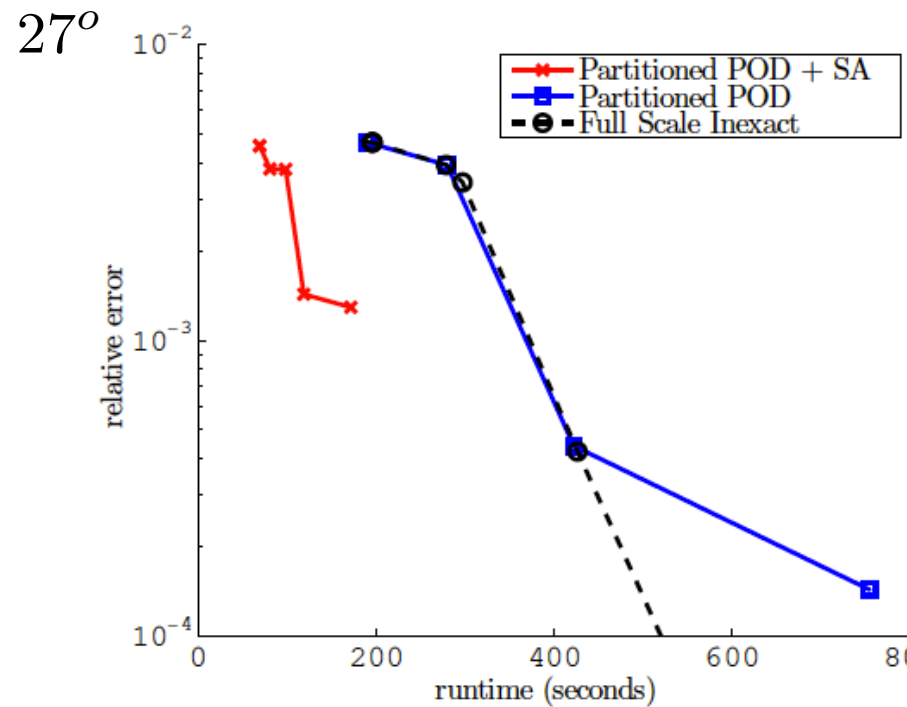
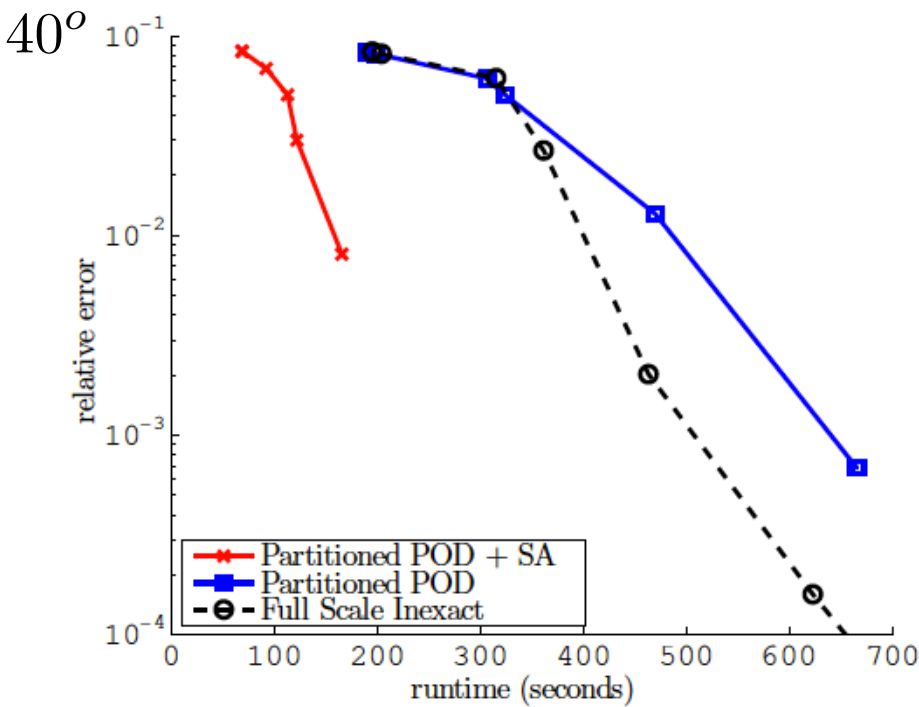


(c) Relative error for the different models using 441 nodes per subdomain

(c) Relative error for the different models using 441 nodes per subdomain

● Relative error

$$\nu^{\text{app},(\mu)}(\underline{\mathbf{U}}^{\text{app}})^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{app}}(t_n, \mu) - \underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|\underline{\mathbf{U}}^{\text{ex}}(t_n, \mu)\|_2^2}$$

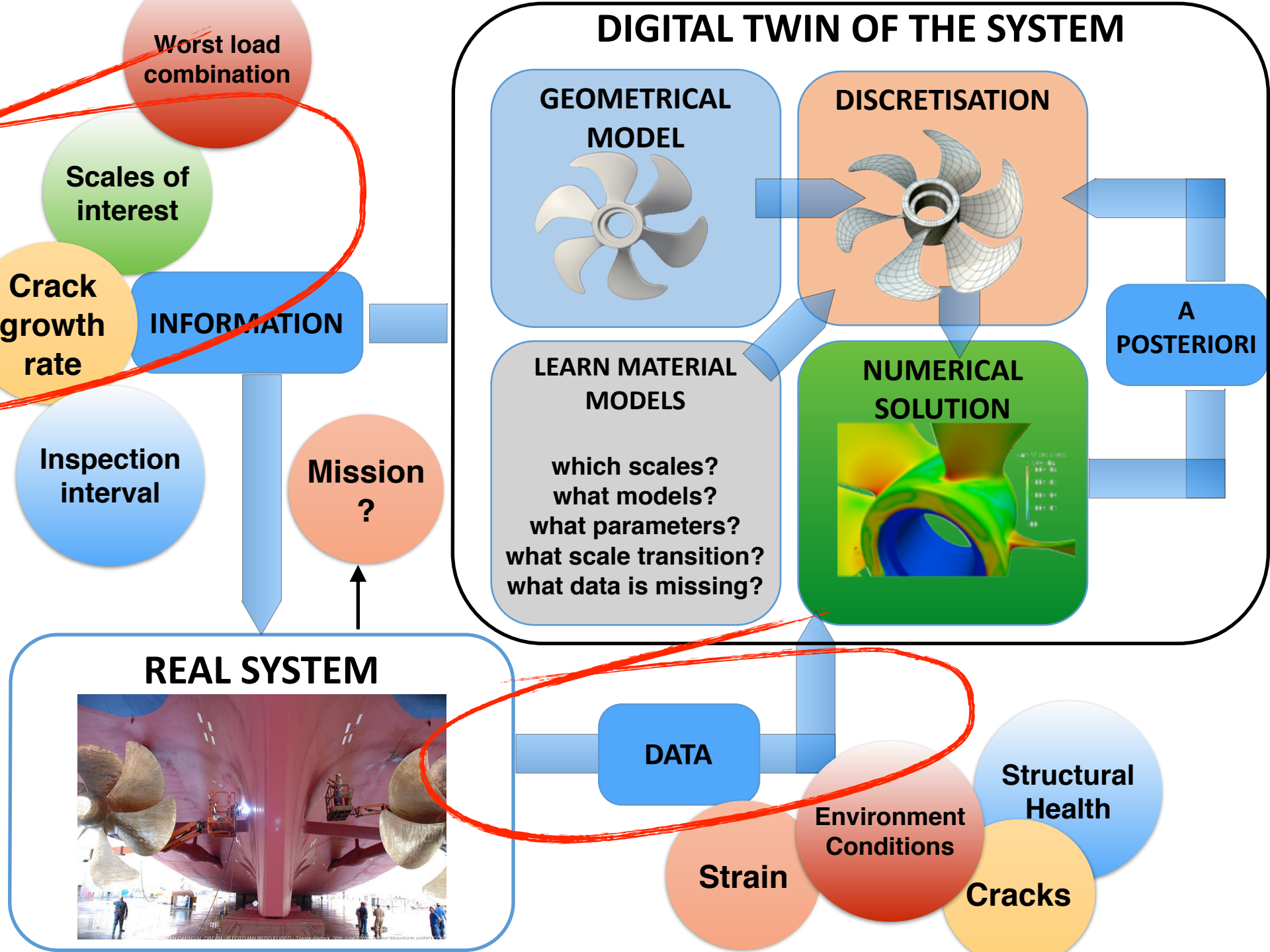


(d) Relative error for the different models using 961 nodes per subdomain

(d) Relative error for the different models using 961 nodes per subdomain

- Domain coupling using the primal Schur-complement domain decomposition method.
- Local subproblems have been reduced by projection in low-dimensional subspaces obtained by the snapshot POD.
- This approach permits to flexibly reduce the computational cost associated with highly nonlinear problems. In particular:
 - ▶ the **local reduced spaces are generated independently**, and have independent dimensions, which allows us to focus the numerical effort where it is most needed.
 - ▶ subdomains that are close to highly damaged zones need a richer model to account for the effect of topological changes. The local **POD transforms automatically generate local reduced spaces of larger dimension in these zones**.
 - ▶ the domain decomposition framework enables us to **switch from reduced local solvers to full local solvers** in a transparent manner. This is particularly useful for the subdomains that contain process zones, as a solution obtained by projection would be more expensive than a direct solution for a desirable accuracy.
 - ▶ the transition between "offline" and "online" computations becomes flexible. The **reduced models can be used in the zones where the local reduced spaces converge quickly** when enriching the snapshot space, while still computing snapshots and refining the reduced models via a direct local solver in the remaining subdomains.

- Further work related to domain decomposition
 - ▶ **load balancing** mismatch would occur when using such a strategy in parallel. CPUs which support domains that are not reduced, or domains for which the corresponding subproblems need to be projected in a space of relatively high dimension, would require to perform more operations. The domain partitioning itself should be performed jointly with the model reduction in order to distribute the load evenly.
 - ▶ **the interface problem itself was not reduced** here, to guarantee the interface kinematic compatibility.
 - ➡ Suboptimal reduced order model. Would generate expensive communications in parallel
 - ➡ A reduction of the interface problem using the POD can be done but is neither elegant nor easy
 - ➡ Dual Schur-complement domain decomposition method would allow the kinematic approximation of the subproblems to include the interface. However, this would only deflect the difficulty to the necessary reduction of the interface Lagrange multiplier space. This issue is our current direction of research.



Worst load combination

Scales of interest

Crack growth rate

INFORMATION

Inspection interval

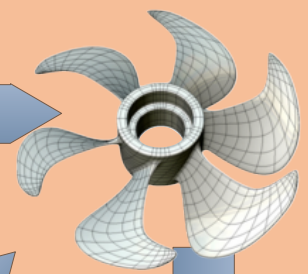
Mission ?

DIGITAL TWIN OF THE SYSTEM

GEOMETRICAL MODEL



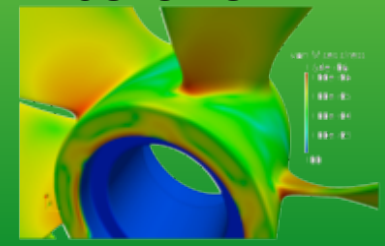
DISCRETISATION



LEARN MATERIAL MODELS

which scales?
what models?
what parameters?
what scale transition?
what data is missing?

NUMERICAL SOLUTION



A POSTERIORI

REAL SYSTEM



DATA

Strain

Environment Conditions

Cracks

Structural Health

Reducing the mesh burden in computational fracture mechanics



Part 0. Enrichment of the finite element method

Skip



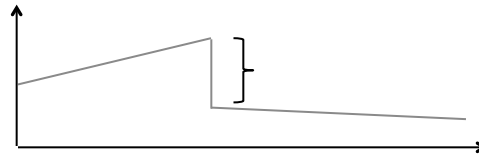
Enrichment

- When the standard finite element method is unable to efficiently reproduce certain features of the sought solution:
 1. Discontinuities - *cracks, material interfaces*
 2. Large gradients - *yield lines, shock waves*
 3. Singularities - *notches, cracks, corners*
 4. Boundary layers - *fluid-fluid, fluid-solid*
 5. Oscillatory behavior - *vibrations, impact*
- The approximation space can be extended by introducing of an *a priori* knowledge about the sought solution, and thereby:
 1. Rendering the mesh independent of any phenomena
 2. reducing error of the approximation locally and globally
 3. improving convergence rates

Classification of discontinuities

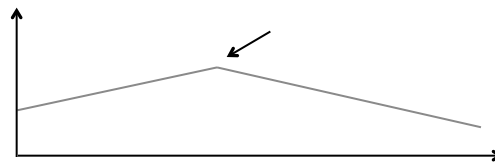
Strong discontinuities

- The primal field of the solution is discontinuous, e.g. cracks lead to strong discontinuities in the displacement field.



Weak discontinuities

- The first derivative of the solution is discontinuous, e.g. discontinuities in the strain field through a material interface.



Classification of enrichments

Global enrichment

- The enrichment is employed on the global level, over the **entire domain**.
- Useful for problems that can be considered as **globally non-smooth** e.g. high-frequency solutions (Helmholtz equation)

Local enrichment

- This enrichment scheme is adopted locally, over a **local subdomain**.
- Useful for problems that only involve **locally non-smooth** phenomena, e.g. solutions with discontinuities.

Classification of enrichments

Extrinsic enrichment

- Associated with additional degrees of freedom and additional shape functions to augment the standard approximation basis.
 1. Extended finite element method (XFEM) - Moës et al. (1999)
 2. Generalised finite element method (GFEM) - Strouboulis et al. (2000a)
 3. Enriched element free Galerkin - Ventura et al. (2002)
 4. *hp* – clouds (Meshless/Hybrid) - Duarte and Oden (1996)

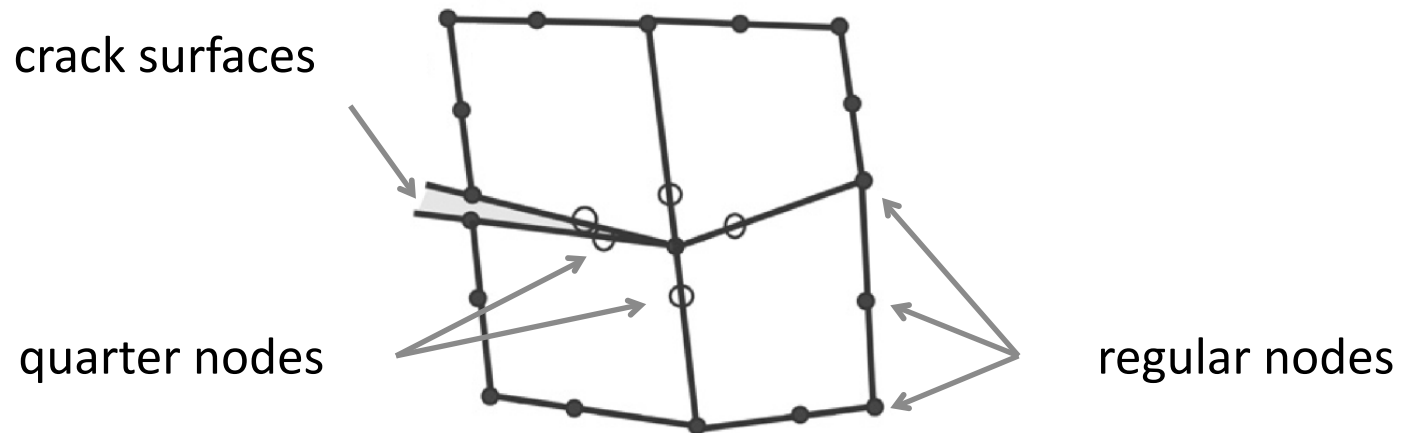
Intrinsic enrichment

- Not accompanied by additional degrees of freedom. Instead, some standard functions are replaced with special (problem specific) functions.
 1. Enriched moving least squares (Meshless) - Fleming et al. (1997)
 2. Enriched weight function (Meshless) - Duflot et al. (2004b)
 3. Intrinsic partition of unity methods - Fries, Belytschko (2006)
 4. Elements with embedded discontinuities

Singular elements (Barsoum, 1974)

For simulating the crack tip singular field in LEFM

- A simple way how to introduce a singularity of $1/\sqrt{r}$ in isoperimetric finite elements is by displacing the mid-side nodes of two adjacent edges to one quarter of the element edge length from the node where the singularity is desired.



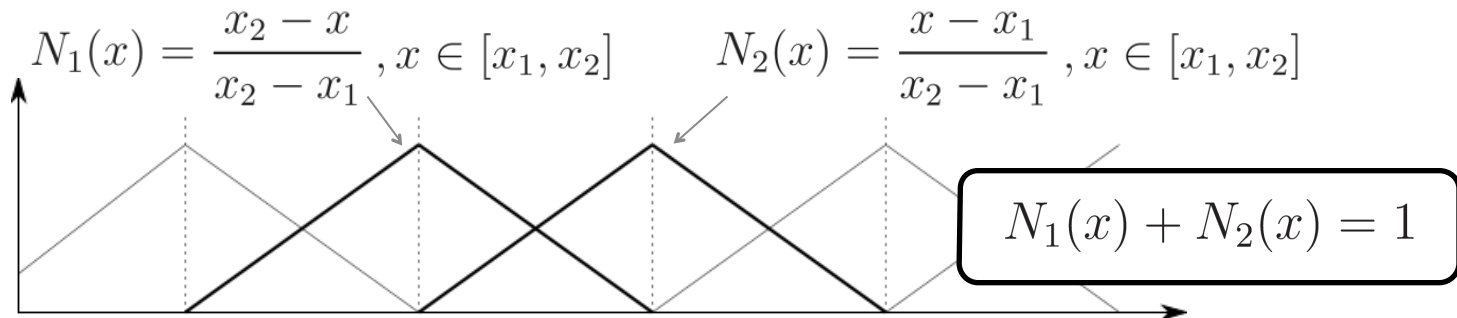
Partition of unity finite element method (PUFEM)

Partition of unity (PU)

- A set of functions ϕ_i whose sum at any point \mathbf{x} inside a domain Ω is equal to unity:

$$\forall \mathbf{x} \in \Omega, \mathbf{x} : \sum_{I=1} \phi_I(\mathbf{x}) = 1$$

- Example PU functions are the finite element “hat” functions:



Reproducibility of PU

- Any function $p(\mathbf{x})$ can be reproduced by a product of that function and the partition of unity functions:

$$\sum_{I=1} \phi_I(\mathbf{x}) p(\mathbf{x}) = p(\mathbf{x})$$

- The function can be adjusted if the sum is modified by introducing parameters q_I :

$$\sum_{I=1} \phi_I(\mathbf{x}) p(\mathbf{x}) q_I = \bar{p}(\mathbf{x})$$

- Reproducibility of $p(\mathbf{x})$ can be controlled and localised to arbitrary regions where $q_I \neq 0$

Partition of unity finite element method (PUFEM)

Formulation of PUFEM (example)

- Find the solution to the following 1D boundary value problem (BVP):

$$\forall x \in [0, l] : \frac{d^2 u}{dx^2} + f = 0$$

$$\text{with BC : } u(0) = 0, u(l) = u_l$$

- If we define two bilinear forms:

$$a(w, u) = \int_0^l \frac{dw}{dx} \frac{du}{dx} dx \quad (w, f) = \int_0^l w f dx$$

- The discrete variational problem can be stated as:

find $u^h \in U^h$ satisfying the BC such that for all $w^h \in W^h$:

$$a(w^h, u^h) = (w^h, f)$$

Partition of unity finite element method (PUFEM)

Formulation of PUFEM (example)

- The approximation/trial function in PUFEM:

$$u^h(x) = \underbrace{\sum_{I=1} N_I(x) u_I}_{\text{standard FE}} + \underbrace{\sum_{J=1} \phi_J(x) \psi(x) q_J}_{\text{PU enriched}}$$

- By choosing $w^h = \delta u^h$, leads to the discrete system of equations:

$$a(\delta u^h, u^h) = (\delta u^h, f)$$

$$\begin{array}{c}
 \mathbf{K}_{ij}^{se} = \int_0^l \frac{dN_i}{dx} \frac{d(\phi_j \psi)}{dx} dx \\
 \mathbf{K}_{ij}^{ss} = \int_0^l \frac{dN_i}{dx} \frac{dN_j}{dx} dx \\
 \mathbf{K}_{ij}^{es} = \int_0^l \frac{d(\phi_i \psi)}{dx} \frac{dN_j}{dx} dx \\
 \mathbf{K}_{ij}^{ee} = \int_0^l \frac{d(\phi_i \psi)}{dx} \frac{d(\phi_j \psi)}{dx} dx
 \end{array}
 \quad \Downarrow \quad
 \begin{array}{c}
 f_i^s = \int_0^l N_i f_x dx \\
 f_i^e = \int_0^l (\phi_i \psi) f_x dx
 \end{array}$$

$$\begin{bmatrix} \mathbf{K}^{ss} & \mathbf{K}^{se} \\ \mathbf{K}^{es} & \mathbf{K}^{ee} \end{bmatrix}
 \begin{Bmatrix} \mathbf{u}^s \\ \mathbf{q}^e \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}^s \\ \mathbf{f}^e \end{Bmatrix}$$

Partition of unity finite element method (PUFEM)

Remarks

- Allows to introduce an arbitrary function $\psi(\mathbf{x})$ in the approximation space by splitting the approximation into a **standard** and **enriched** parts.
- Enrichment can be **localised** to a small region around the features of interest – computationally advantageous.
- Provides a systematic means of introducing multiple enrichments.

References:

- Melenk and Babuska (1996)
- Duarte and Oden (1996)

The Generalised Finite Element Method (GFEM)

GFEM

- Originally associated with global PU enrichment
- Shape functions in the enriched part are usually different from the shape functions in the standard part i.e. $\phi_I(x) \neq N_I(x)$
- Introduced numerically generated enrichment functions, e.g. a solution in the vicinity of a bifurcated crack as enrichment

References:

- Melenk (1995)
- Melenk and Babuška (1996)
- Strouboulis et al. (2000)

The Extended Finite Element Method (XFEM)

XFEM

- Associated with local discontinuous PU enrichment e.g.:
 - a. propagation of cracks
 - b. evolution of dislocations
 - c. phase boundaries
- Both GFEM and XFEM are essentially identical in their application, i.e. extrinsic PU enrichment

References:

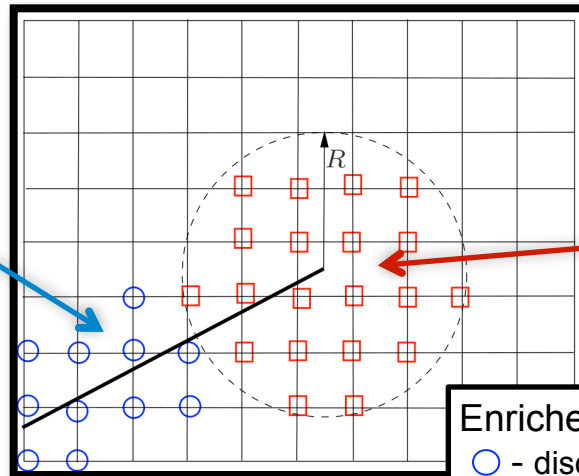
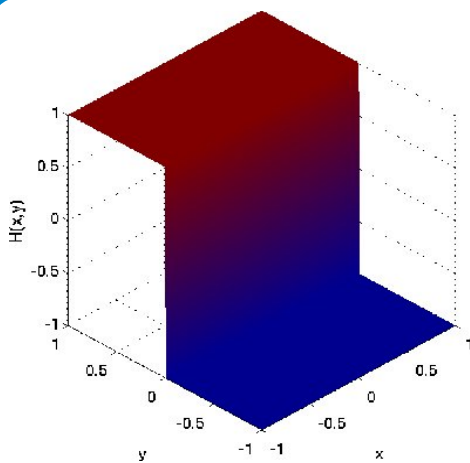
- Belytschko and Black (1999)
- Moës et. al. (1999)
- Dolbow (1999)

Formulation for crack growth:

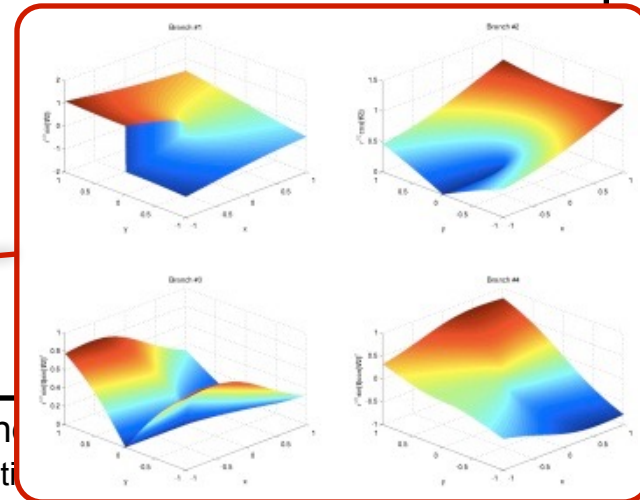
$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) \mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K \in \mathcal{N}_K} N_K(\mathbf{x}) \sum_{\alpha=1}^4 f_\alpha(\mathbf{x}) \mathbf{b}^{K\alpha}}_{\text{singular tip enrichment}}$$

$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above crack} \\ -1 & \text{if } \mathbf{x} \text{ below crack} \end{cases}$$

$$\{f_\alpha(r, \theta), \alpha = 1, 4\} = \left\{ \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2} \sin \theta, \sqrt{r} \cos \frac{\theta}{2} \sin \theta \right\}$$



Enriched nodes
 ○ - discontinuous
 □ - singular





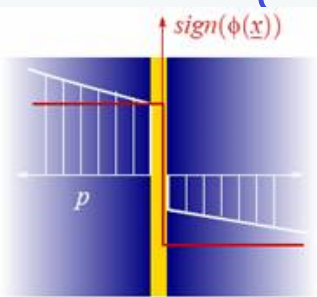
$$u_i^h(\mathbf{x}) = \sum_{n_I \subset N} N_I(\mathbf{x}) u_{iI} + \sum_{n_J \subset N^c} N_J(\mathbf{x}) a_{iJ} H(\mathbf{x}) + \sum_{n_K \subset N^f} \phi_K(\mathbf{x}) b_{iK} \Psi(\mathbf{x})$$

classical
enriched

$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above} \\ -1 & \text{if } \mathbf{x} \text{ below} \end{cases}$$

Heaviside function

Asymptotic fields



$$\psi(r, \theta) = \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \sin \theta \sin \frac{\theta}{2}, \sqrt{r} \sin \theta \cos \frac{\theta}{2}$$

$$u_i^h(\mathbf{x}) = \sum_{n_I \subset N} N_I(\mathbf{x}) u_{iI} + \sum_{n_J \subset N^c} N_J(\mathbf{x}) a_{iJ} H(\mathbf{x}) + \sum_{n_K \subset N^f} \phi_K(\mathbf{x}) b_{iK} \Psi(\mathbf{x})$$

Standard FEM mesh

enriched

Heaviside function

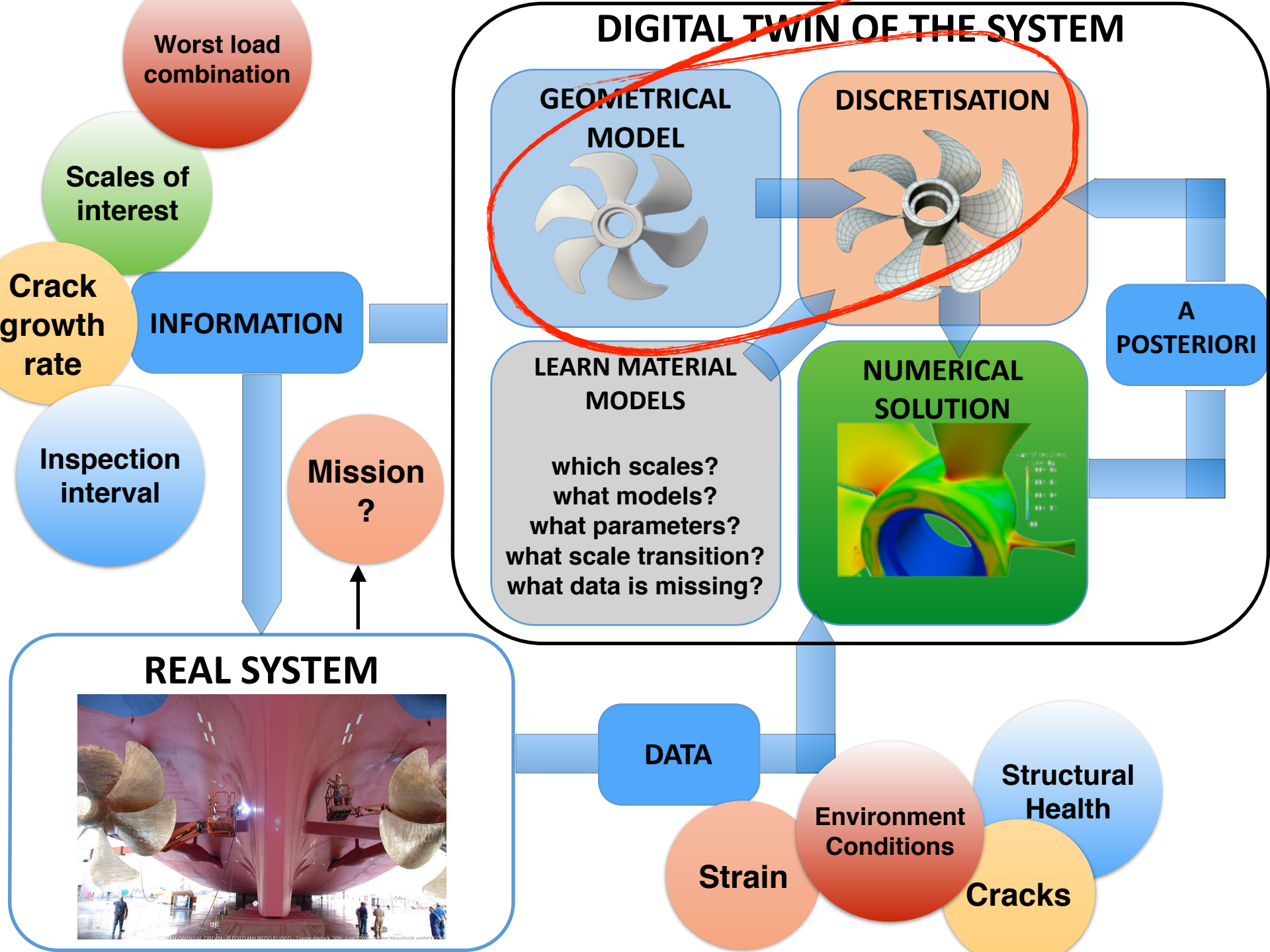
Asymptotic fields

ENRICHED NODES

- Tip
- Interior

- Part I.** Streamlining the CAD-analysis transition
- Part II.** Some advances in enriched FEM
- Part III.** Application to H cutting of Si wafers
- Part IV.** Application to interactive cutting sim.

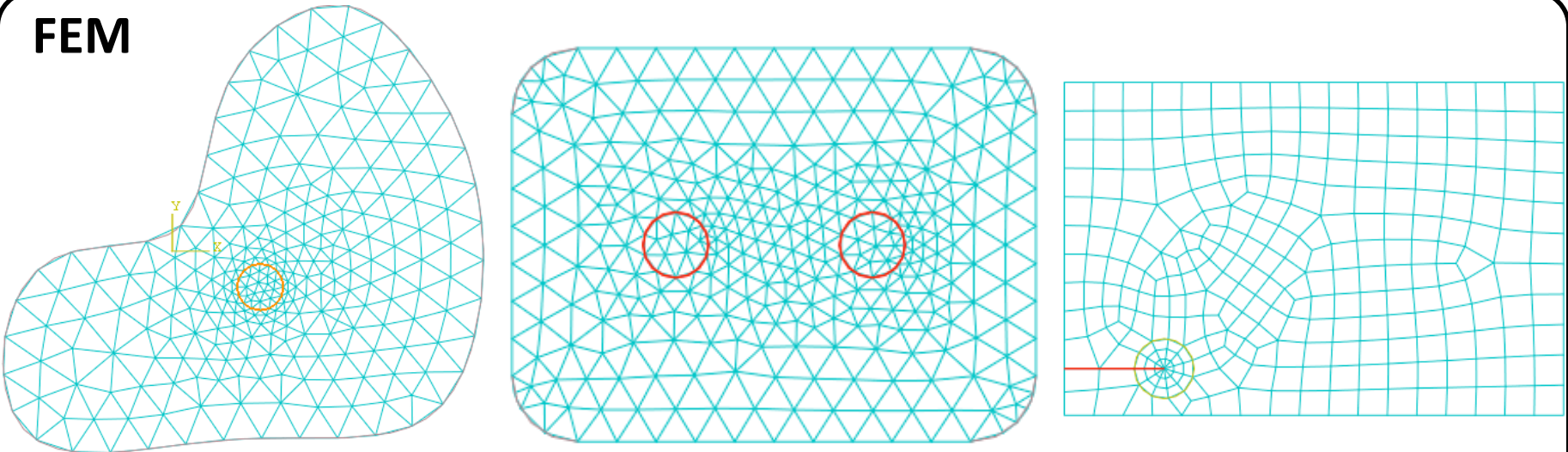
erc



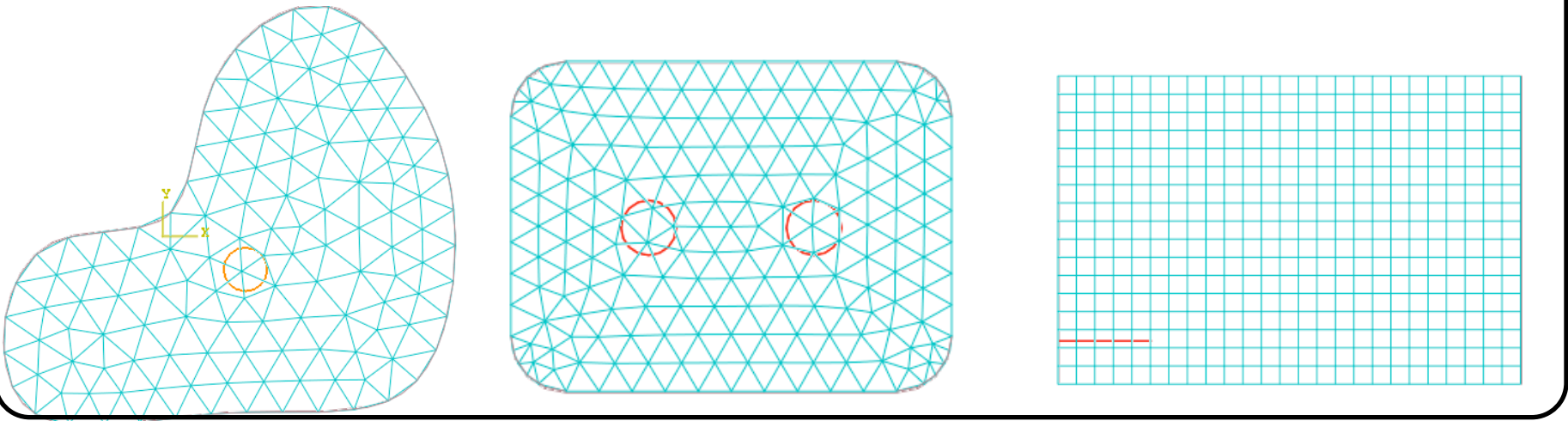
Motivation: free boundary problems - mesh burden



FEM



XFEM



ITN
INSIST

Part I. Streamlining the CAD-analysis transition

Coupling, or decoupling?



Decouple geometry and analysis

- Meshfree methods (Monaghan, 1977, Belytschko, *et al.* 1994)
- PU enrichment (Melenk & Babuška, 1996; Belytschko, *et al.* 1999)
- Immersed boundary method (Mittal, *et al.* 2005)

Improve element formulations (use simplex elements)

- Smoothed FEM (Liu, *et al.* 2006), smoothed XFEM (Bordas,...)
- Polygonal FEM (Alwood, *et al.* 1969)

Boundary discretisation

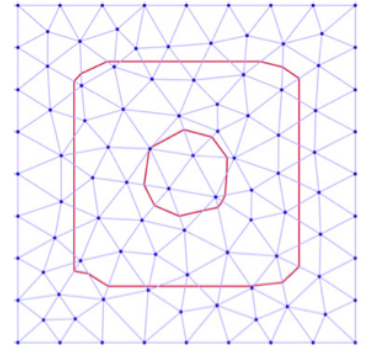
- Boundary element method (Rizzo, 1967)
- Scaled boundary FEM (Song, *et al.* 1997)

Couple geometry and analysis: Isogeometric analysis (Hughes, 2005), Isogeometric BEM (Simpson, *et al.* 2012)

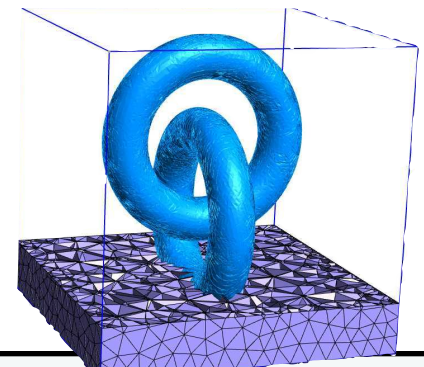
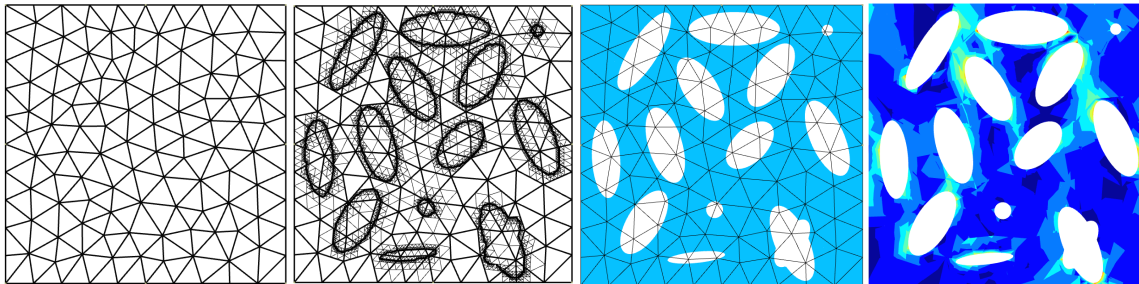
Part I.a. *Decoupling CAD and Analysis.*

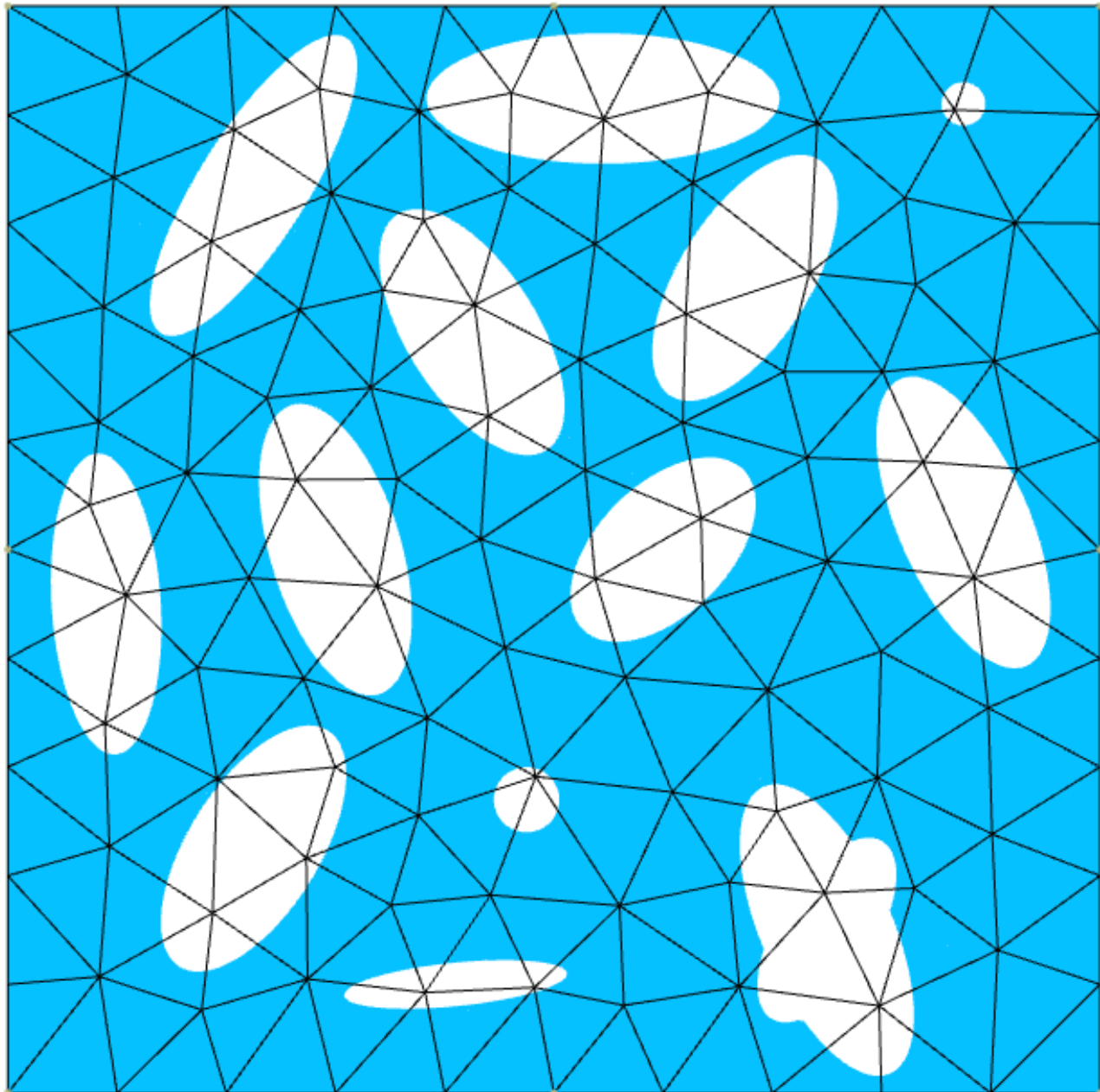
Separate field and boundary discretisation

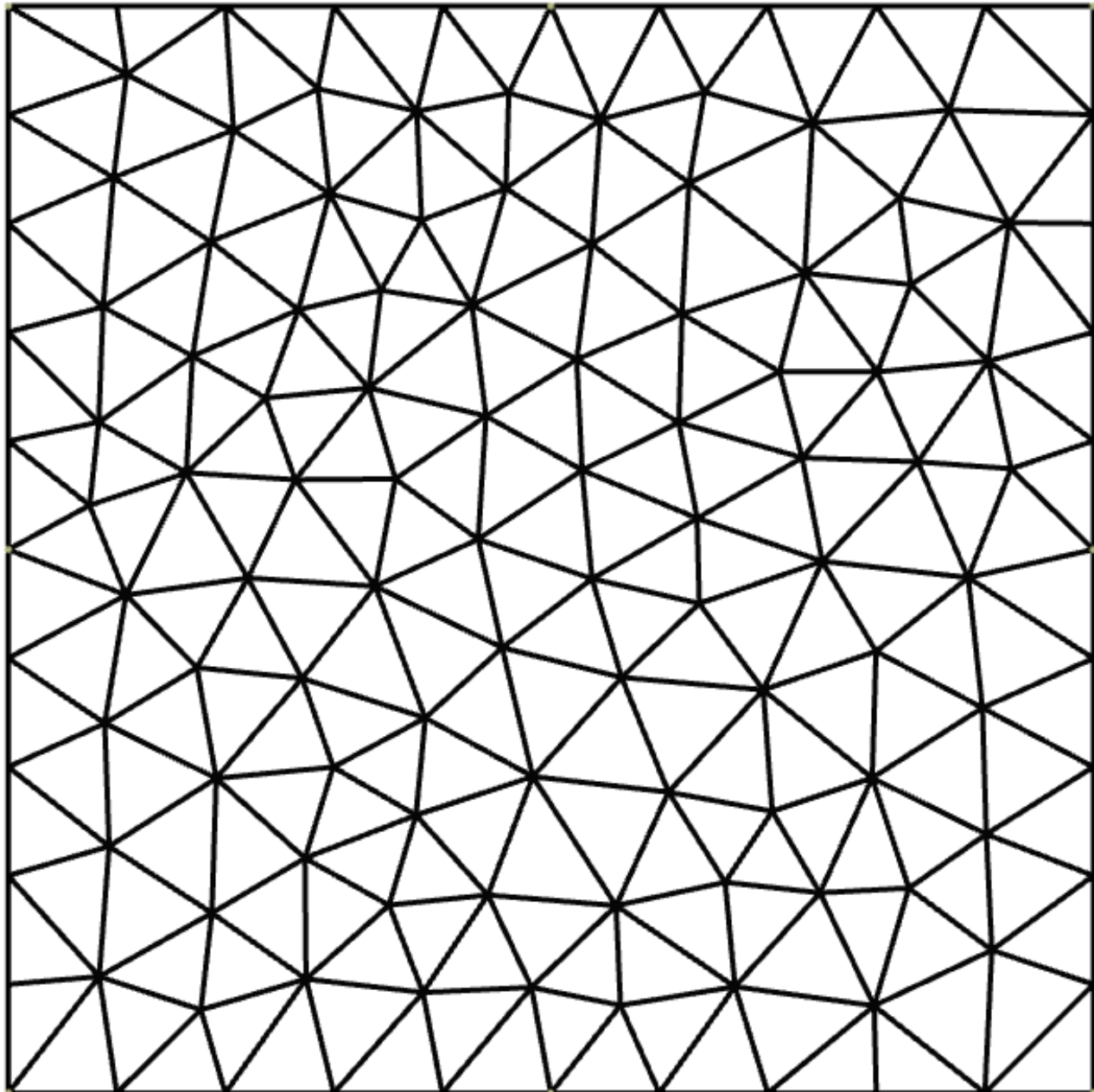
- Immersed boundary method (Mittal, *et al.* 2005)
- Fictitious domain (Glowinski, *et al.* 1994)
- Embedded boundary method (Johansen, *et al.* 1998)
- Virtual boundary method (Saiki, *et al.* 1996)
- Cartesian grid method (Ye, *et al.* 1999, Nadal, 2013)

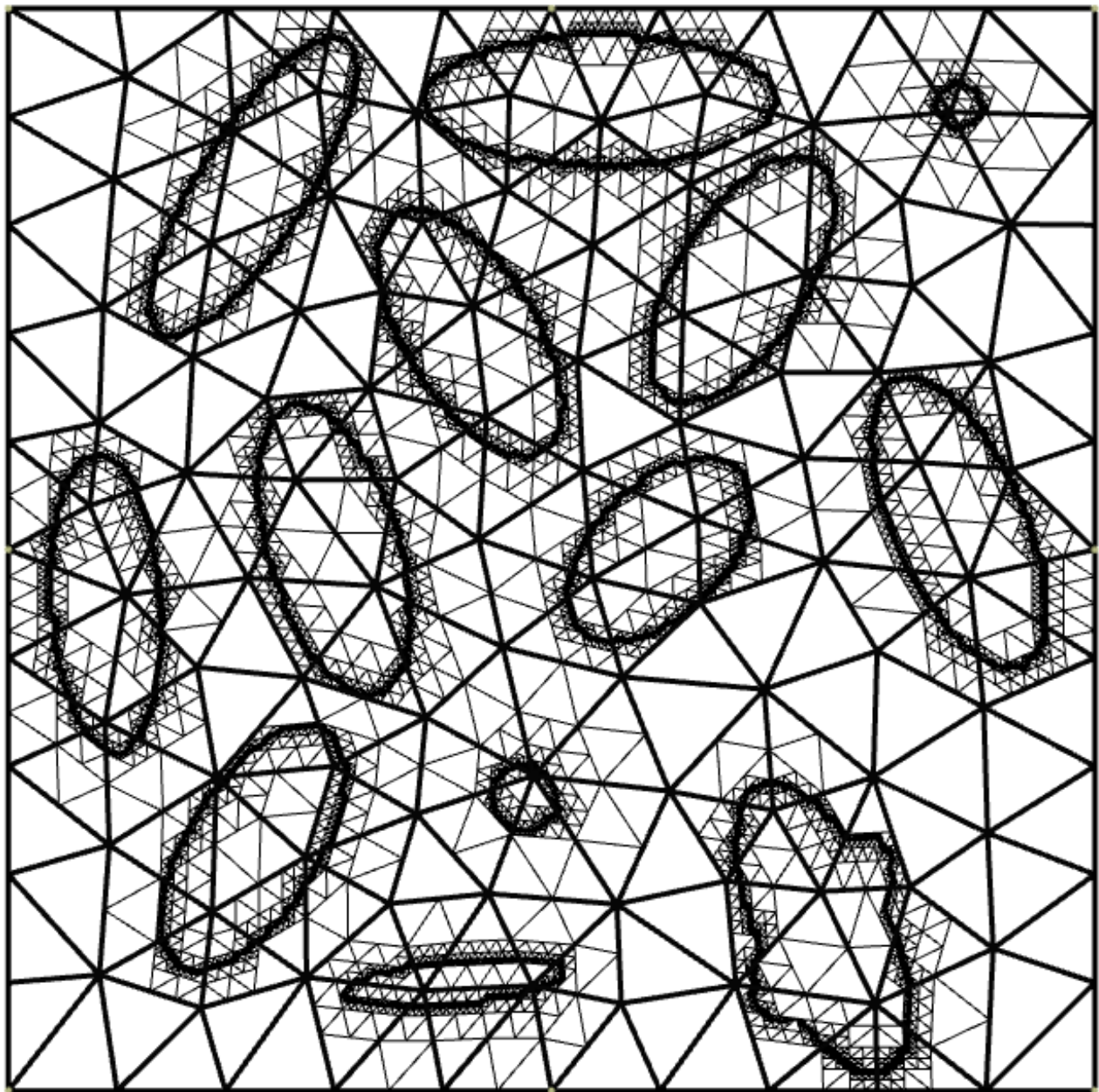


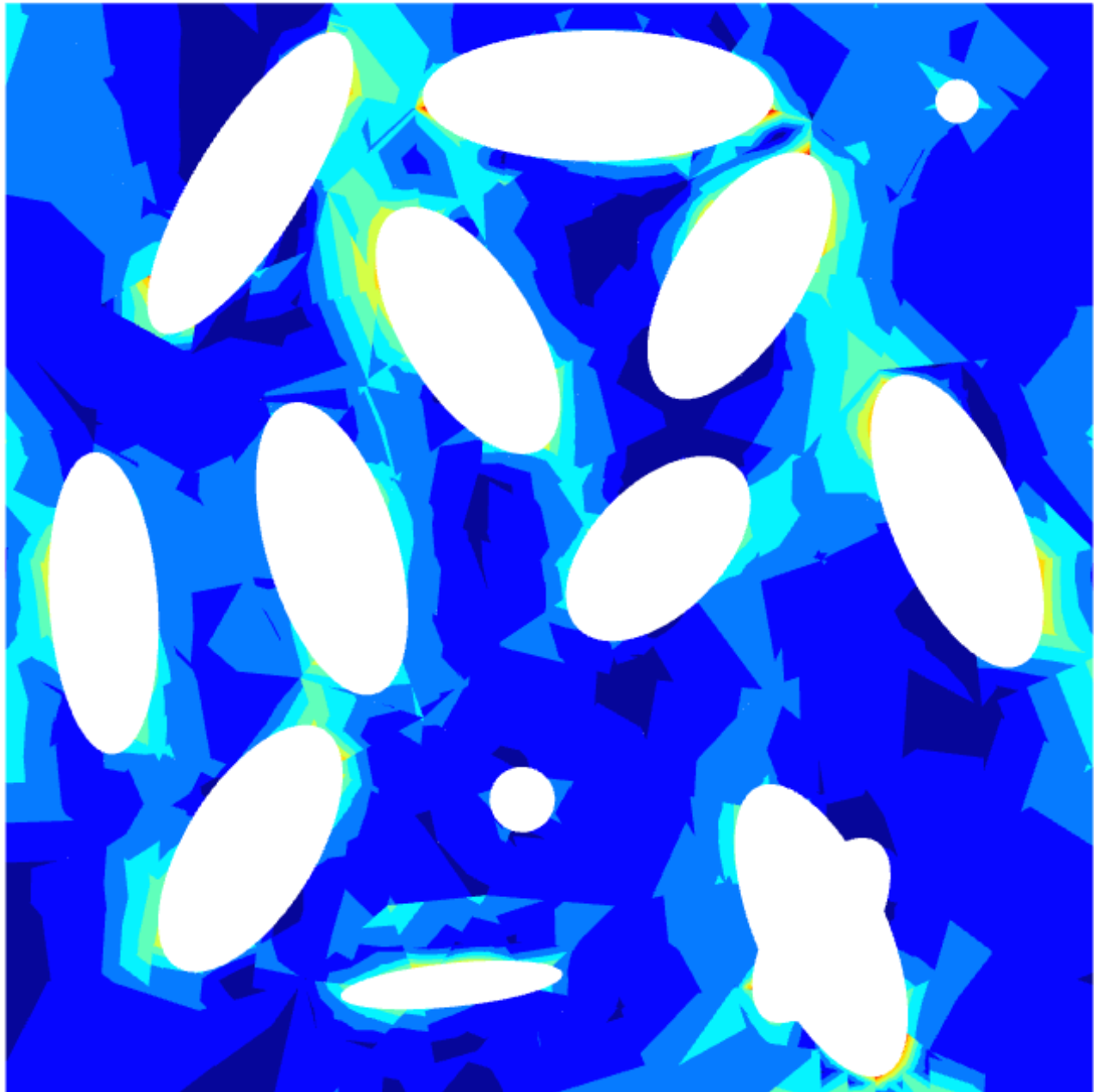
- ✓ Easy adaptive refinement + error estimation (Nadal, 2013)
- ✓ Flexibility of choosing basis functions
- Accuracy for complicated geometries? BCs on implicit surfaces?
- ➔ An accurate and implicitly-defined geometry from arbitrary parametric surfaces including corners and sharp edges (Moumnassi, *et al.* 2011)





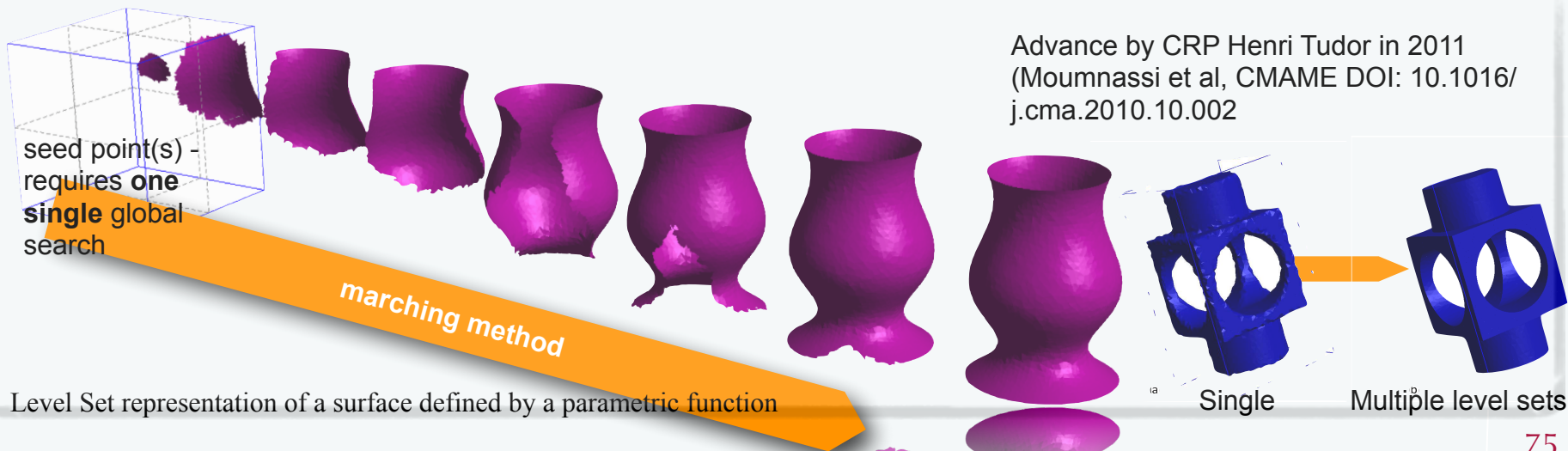
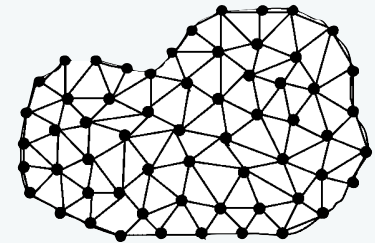
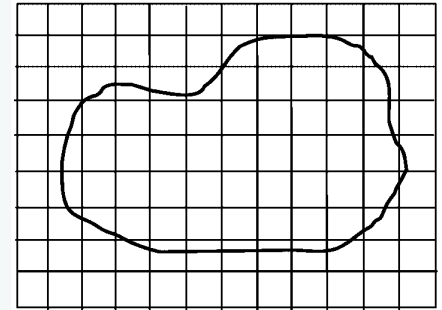






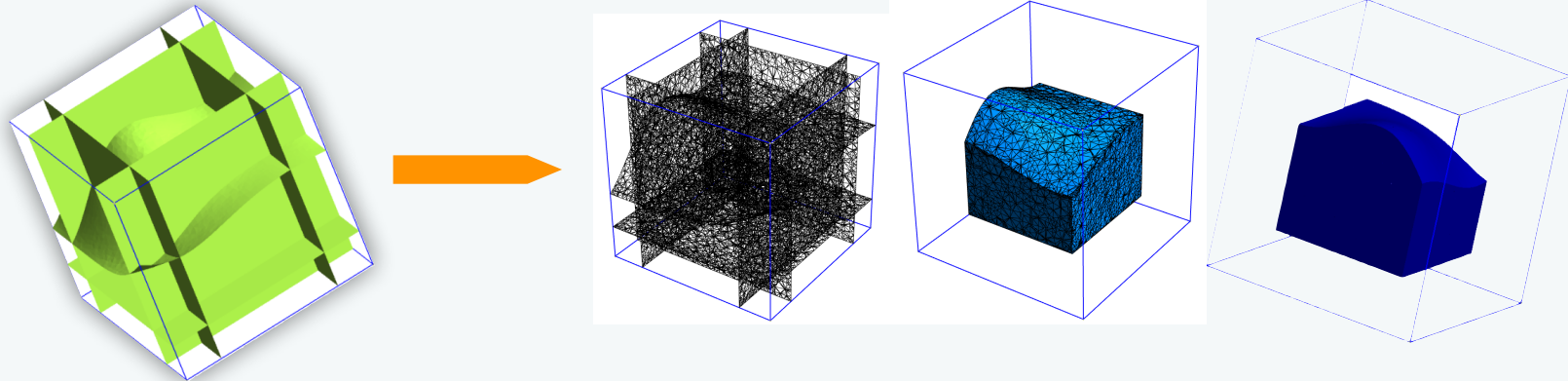
● Objectives

- ▶ insert surfaces in a structured mesh
 - without meshing the surfaces (boundary, cracks, holes, inclusions, etc.)
 - directly from the underlying CAD model
 - model arbitrary solids, including sharp edges and vertices
- ▶ keep as much as possible of the mesh as the CAD model evolves, i.e. reduce mesh dependence of the implicit boundary representation
- ▶ maintain the convergence rates and implementation simplicity of the FEM

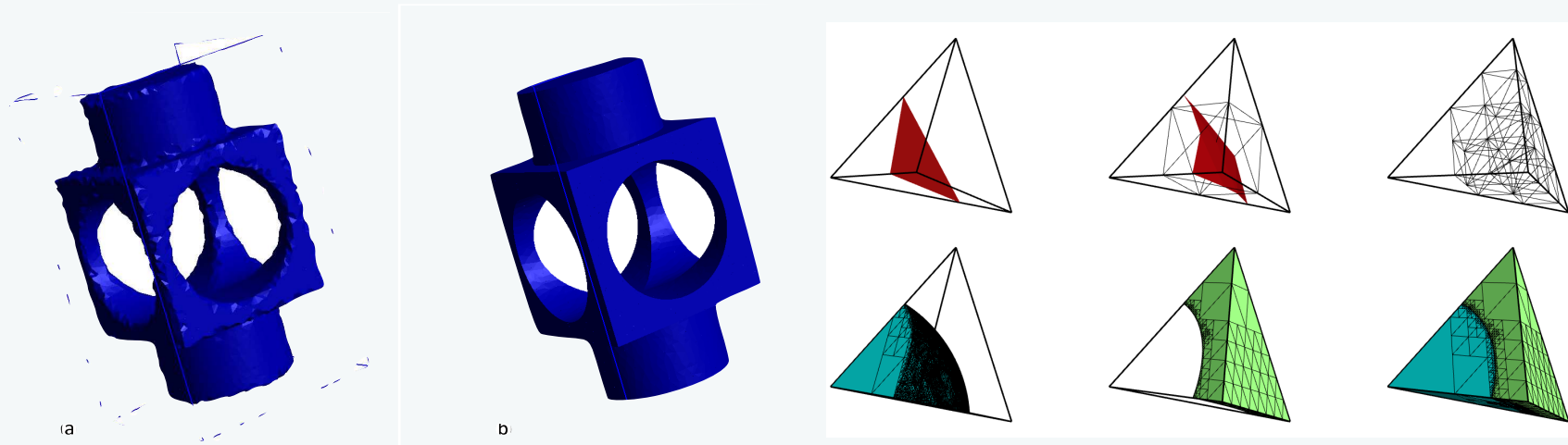


Examples

- multiple level sets



- single (left) versus multiple (right)

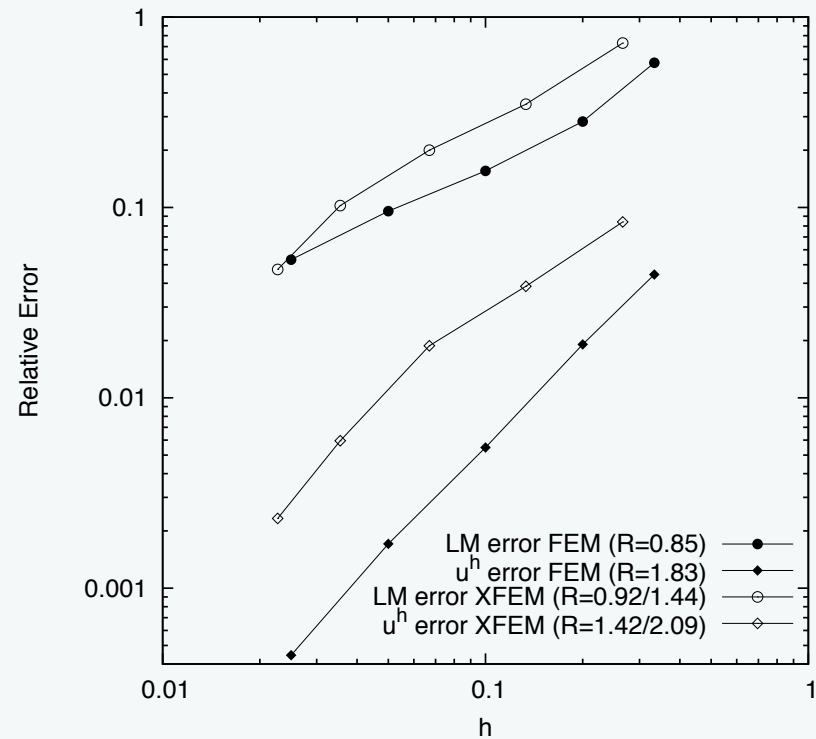
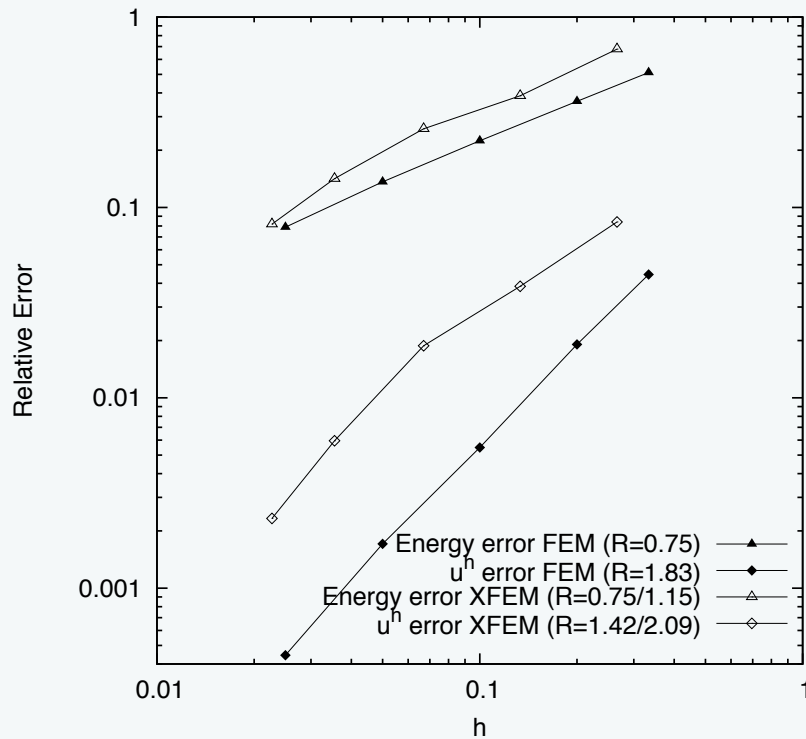
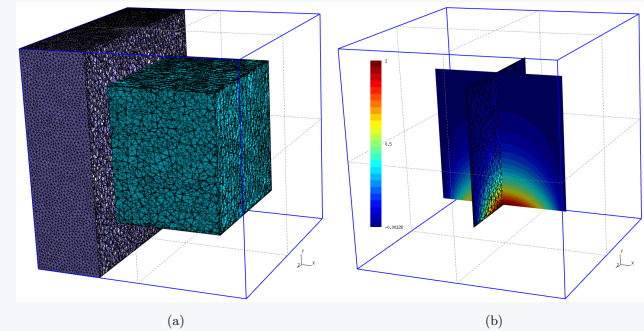


- Laplace equation on a cube

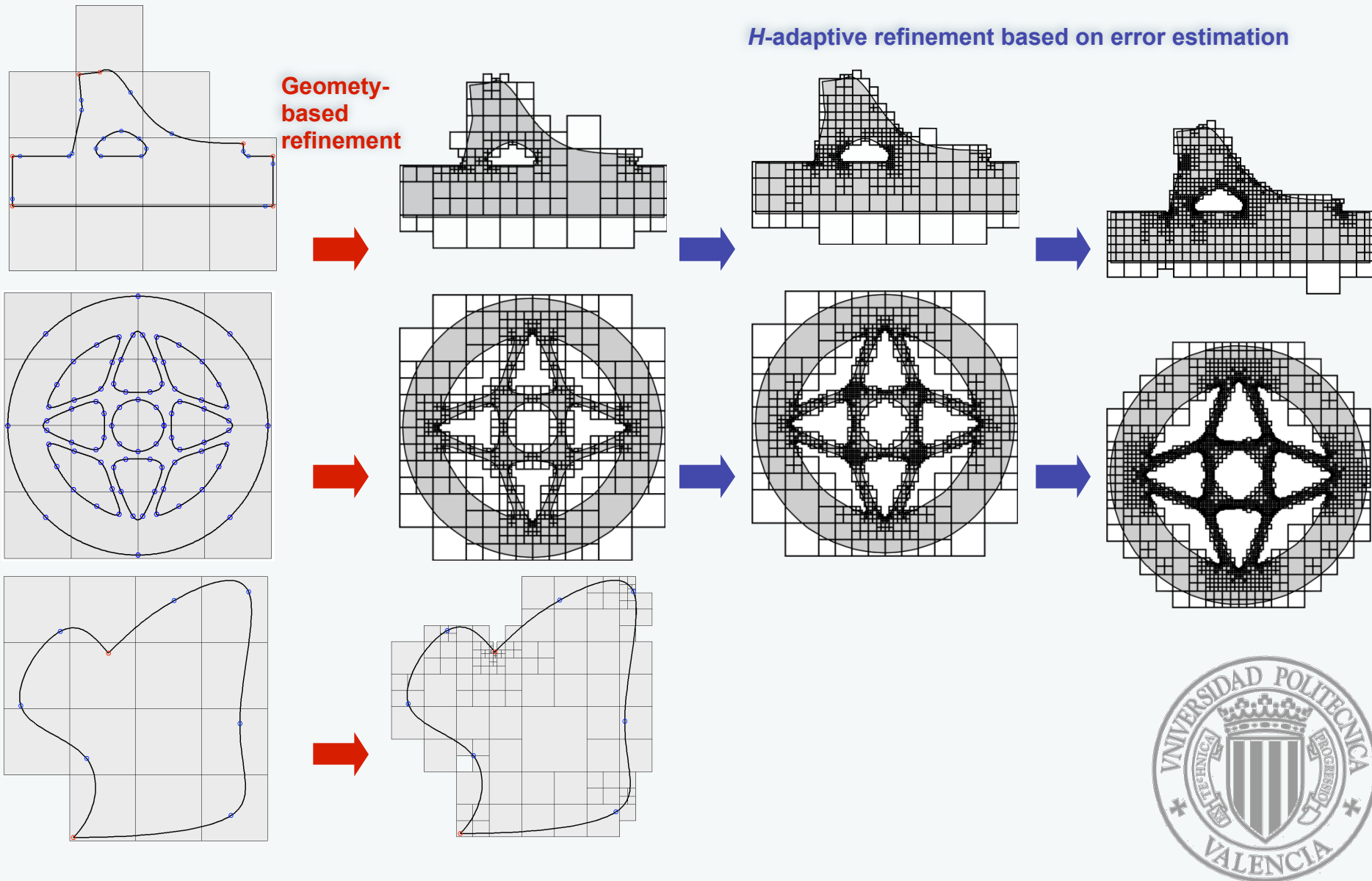
- convergence rates

➔ optimal

➔ requires proper Lagrange multiplier space to eradicate spurious oscillations

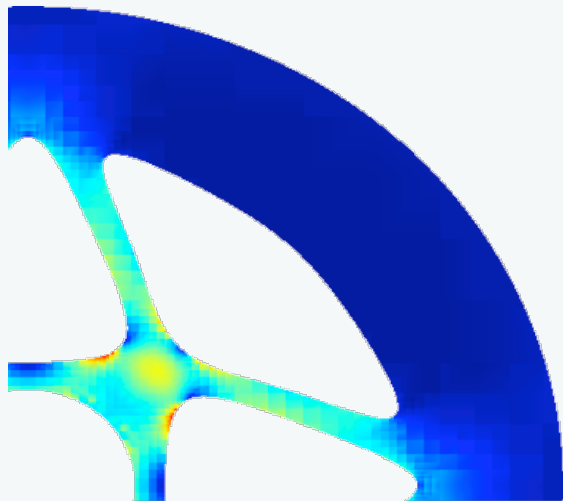


Pixel/Voxel-based FEA on Cartesian grids (Valencia)

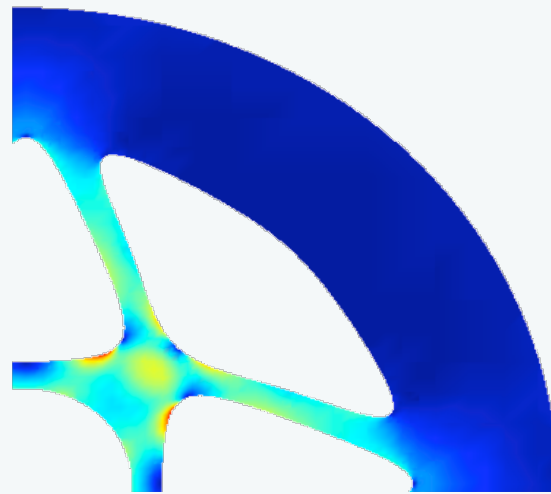


Pixel/Voxel-based FEA on Cartesian grids (Valencia)

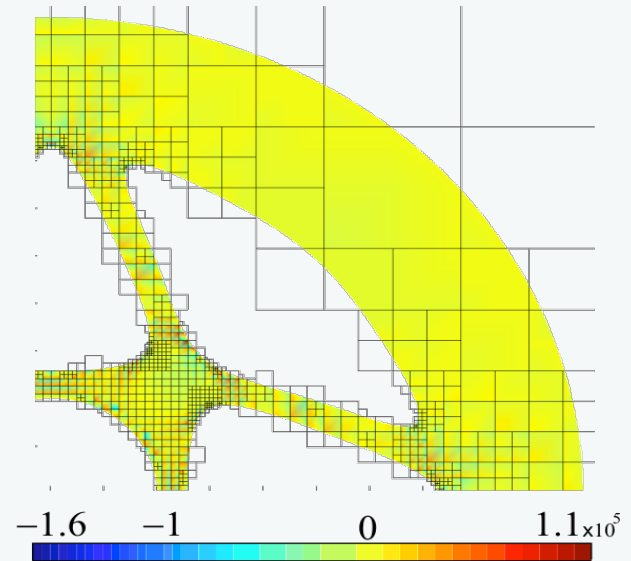
FEM



SPR-C

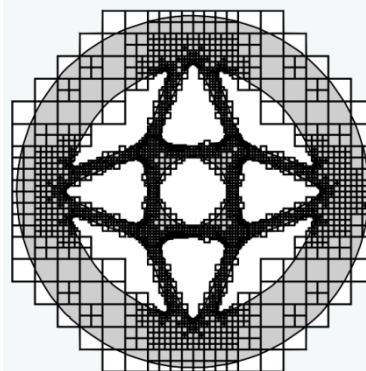
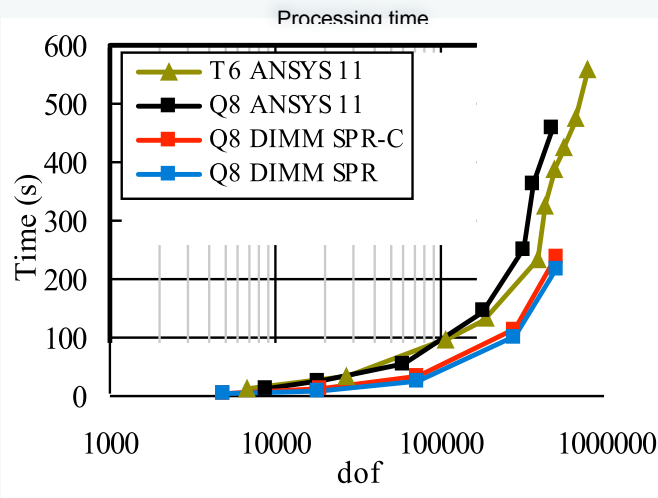


SPR-C-FEM



45

Quad8 uniform refinement



Part I.b. *Coupling CAD and Analysis.*



- P. Kagan, A. Fischer, and P. Z. Bar-Yoseph. New B-Spline Finite Element approach for geometrical design and mechanical analysis. *IJNME*, 41(3):435–458, 1998.
- F. Cirak, M. Ortiz, and P. Schröder. Subdivision surfaces: a new paradigm for thin-shell finite-element analysis. *IJNME*, 47(12): 2039–2072, 2000.
- Constructive solid analysis: a hierarchical, geometry-based meshless analysis procedure for integrated design and analysis. D. Natekar, S. Zhang, and G. Subbarayan. *CAD*, 36(5): 473--486, 2004.
- T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *CMAME*, 194(39-41):4135–4195, 2005.
- J. A. Cottrell, T. J.R. Hughes, and Y. Bazilevs. *Isogeometric Analysis: Toward Integration of CAD and FEA*. Wiley, 2009.



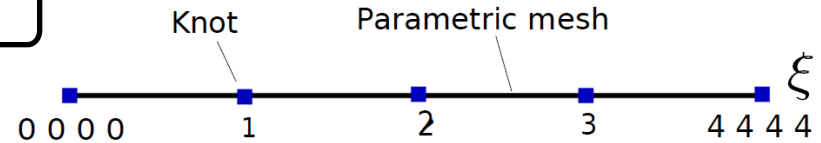
- P. Kagan, A. Fischer, and P. Z. Bar-Yoseph. New B-Spline Finite Element approach for geometrical design and mechanical analysis. *IJNME*, 41(3):435–458, 1998.
- F. Cirak, M. Ortiz, and P. Schröder. Subdivision surfaces: a new paradigm for thin-shell finite-element analysis. *IJNME*, 47(12): 2039–2072, 2000.
- **Constructive solid analysis: a hierarchical, geometry-based meshless analysis procedure for integrated design and analysis.** D. Natekar, S. Zhang, and G. Subbarayan. *CAD*, 36(5): 473--486, 2004.
- **T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement.** *CMAME*, 194(39-41):4135–4195, 2005.
- J. A. Cottrell, T. J.R. Hughes, and Y. Bazilevs. *Isogeometric Analysis: Toward Integration of CAD and FEA*. Wiley, 2009.

Non-uniform rational B-splines

Knot vector

a non-decreasing set of coordinates in the parametric space.

$$\Xi = \{\xi_1, \xi_2, \dots, \xi_{n+p+1}\}$$



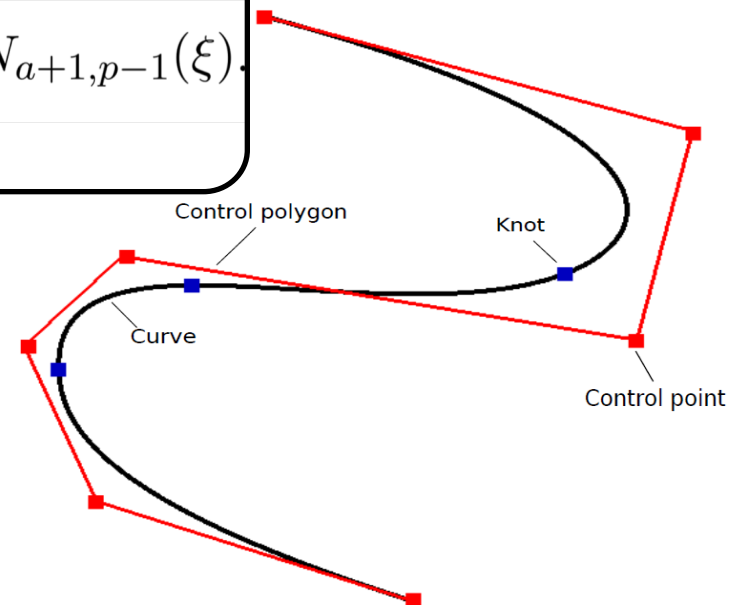
B-spline basis function

$$N_{a,0}(\xi) = \begin{cases} 1, & \text{if } \xi_a \leq \xi < \xi_{a+1} \\ 0, & \text{otherwise.} \end{cases}$$

$$N_{a,p}(\xi) = \frac{\xi - \xi_a}{\xi_{a+p} - \xi_a} N_{a,p-1}(\xi) + \frac{\xi_{a+p+1} - \xi}{\xi_{a+p+1} - \xi_{a+1}} N_{a+1,p-1}(\xi)$$

NURBS basis function

$$R_{a,p}(\xi) = \frac{N_{a,p}(\xi)w_a}{W(\xi)} = \frac{N_{a,p}(\xi)w_a}{\sum_{\hat{a}=1}^n N_{\hat{a},p}w_{\hat{a}}}$$



Properties of NURBS



- Partition of Unity

$$\sum_{i=1}^n R_{i,p}(\xi) = 1$$

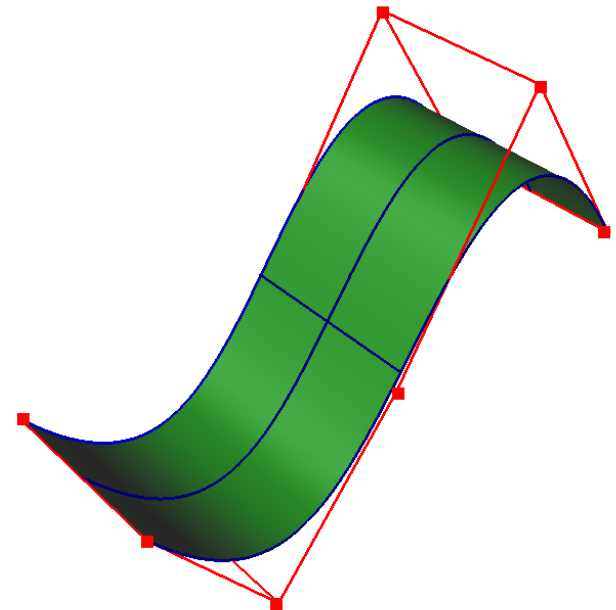
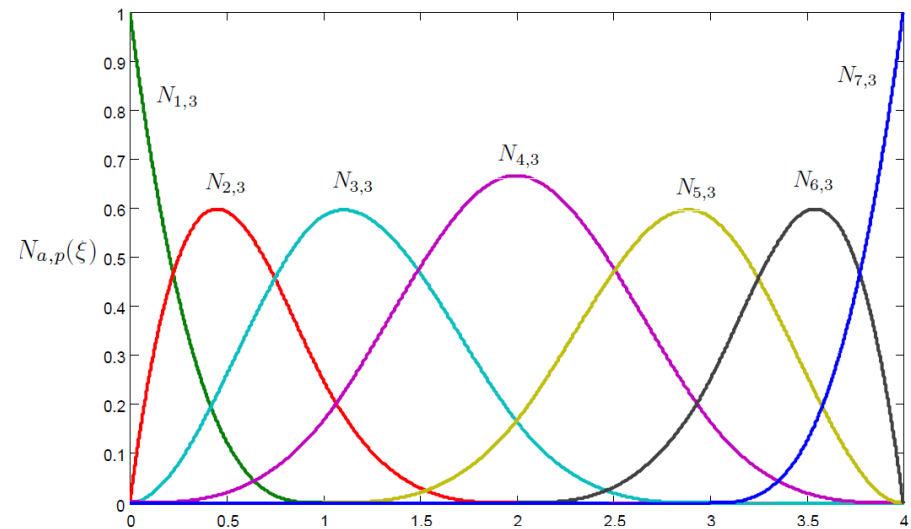
- Non-negative

- $p-1$ continuous derivatives

- Tensor product property

$$S(\xi, \eta) = \sum_{i=1}^n \sum_{j=1}^m R_{i,p}^1(\xi) R_{j,q}^2(\eta) \mathbf{B}_{i,j}$$

$$\sum_{i=1}^n \sum_{j=1}^m R_{i,p}^1(\xi) R_{j,q}^2(\eta) = \left(\sum_{i=1}^n R_{i,p}^1(\xi) \right) \left(\sum_{j=1}^m R_{j,q}^2(\eta) \right)$$



NURBS to T-splines



www.tsplines.com

(NURBS geometry)



www.tsplines.com

(T-splines geometry)

NURBS

- No watertight geometry
- No local refinement scheme

T-splines

- Local knot vector (as Point-based splines)
- Global topology

Y. Bazilevs, V.M. Calo, J.A. Cottrell, J.A. Evans, T.J.R. Hughes, S. Lipton, M.A. Scott, and T.W. Sederberg. Isogeometric analysis using T-splines. CMAME, 199(5-8):229–263, 2010.

Isogeometric Analysis with BEM



1. IGABEM with NURBS for 2D elastic problems (Simpson, *et al.* CMAME, 2011).
2. IGABEM with T-splines for 3D elastic problems (Scott, *et al.* CMAME, 2012).
3. IGABEM with T-splines for 3D acoustic problems (Simpson, *et al.* 2013 - MAFELAP2013 TH1515).

Difficulties in dealing with nonlinear problems and non-homogeneous materials.

IGABEM formulation

Regularised form of boundary integral equation for 2D linear elasticity

$$\int_{\Gamma} \mathbf{T}(\mathbf{s}, \mathbf{x}) [\mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{s})] d\Gamma(\mathbf{x}) = \int_{\Gamma} \mathbf{U}(\mathbf{s}, \mathbf{x}) \mathbf{t}(\mathbf{x}) d\Gamma(\mathbf{x})$$

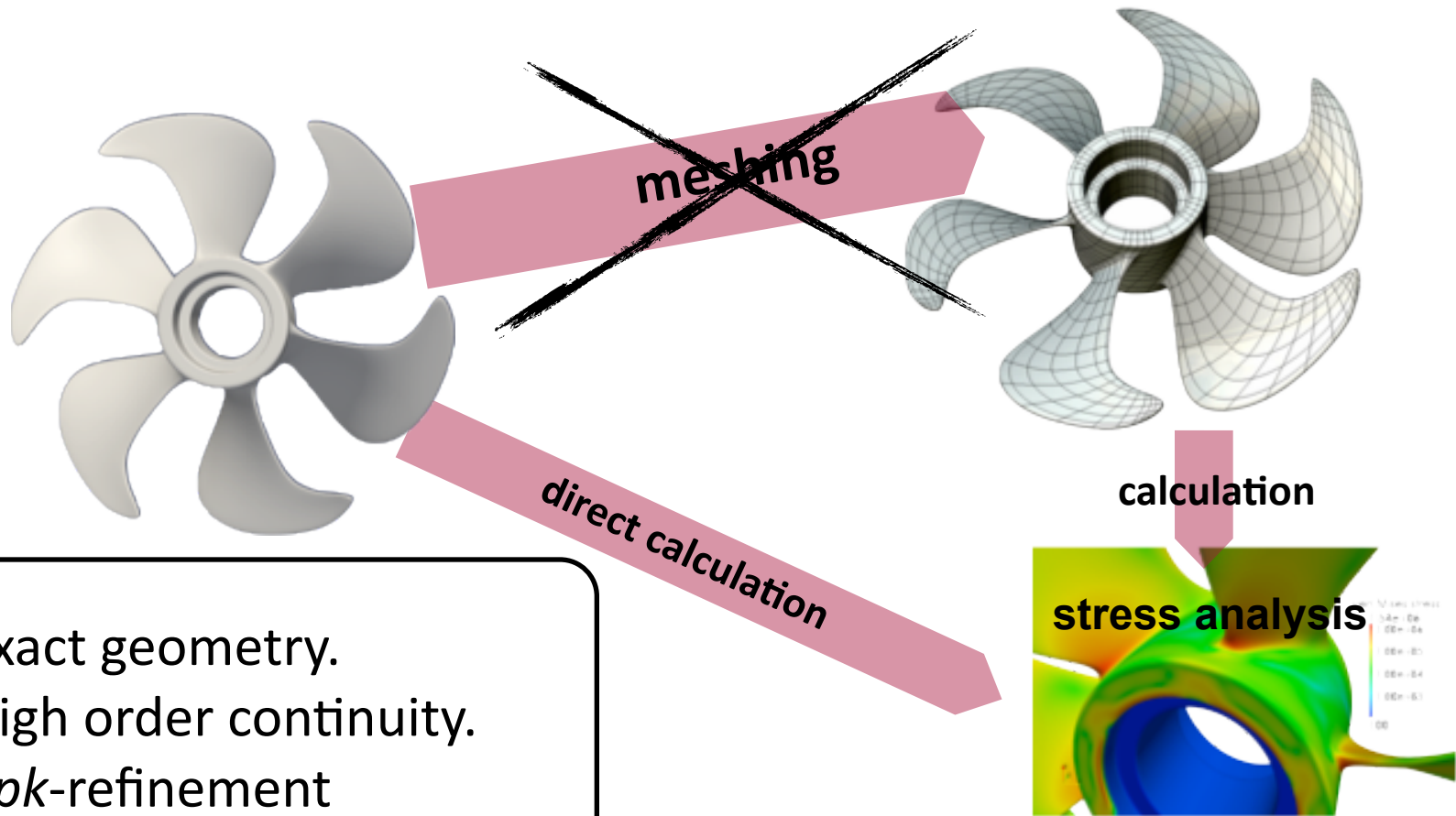
where \mathbf{x} and \mathbf{s} are field point and source point respectively, \mathbf{u} and \mathbf{t} are displacement and traction around the boundary, \mathbf{T} and \mathbf{U} are fundamental solutions.

Discretise the geometry and solution field using NURBS

$$\mathbf{x} = \sum_{A=1}^{n_A} N_A(\xi) \mathbf{B}_A = N_A(\xi) \mathbf{B}_A$$
$$\mathbf{u} = \sum_{A=1}^{n_A} N_A(\xi) \mathbf{u}_A = N_A(\xi) \mathbf{u}_A$$
$$\mathbf{t} = \sum_{B=1}^{n_B} N_B(\xi) \mathbf{t}_B = N_B(\xi) \mathbf{t}_B$$

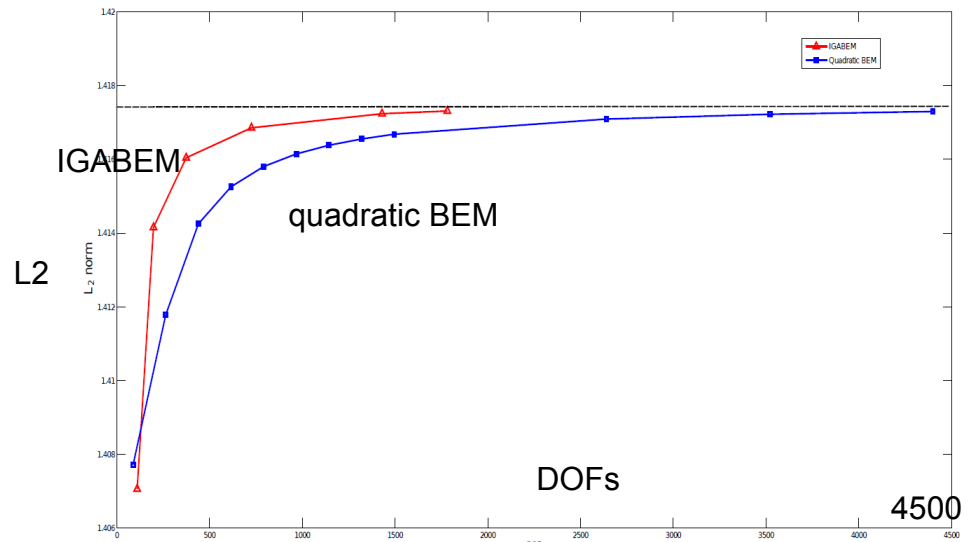
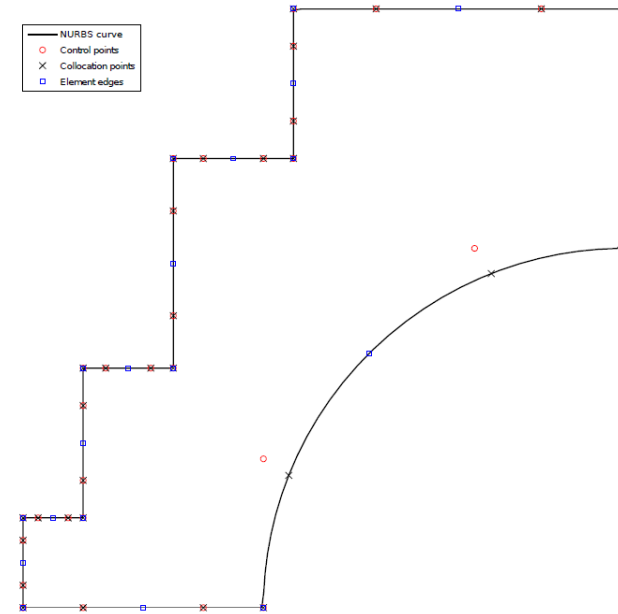
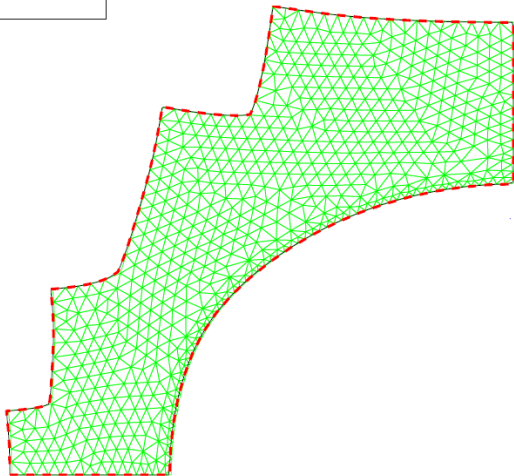
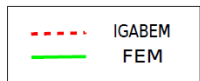
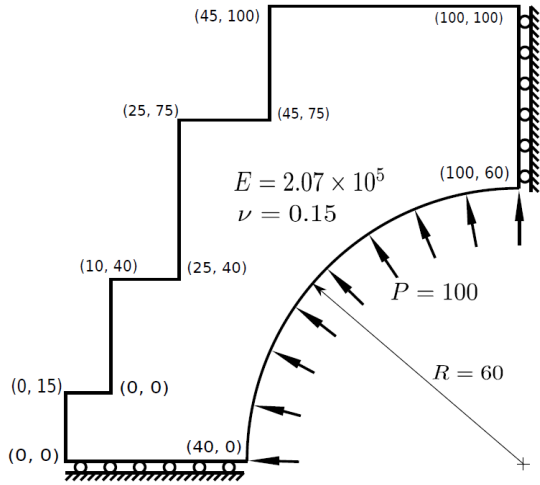


Approximate the unknown fields with the same basis functions (NURBS, T-splines ...) as that used to generate the CAD model

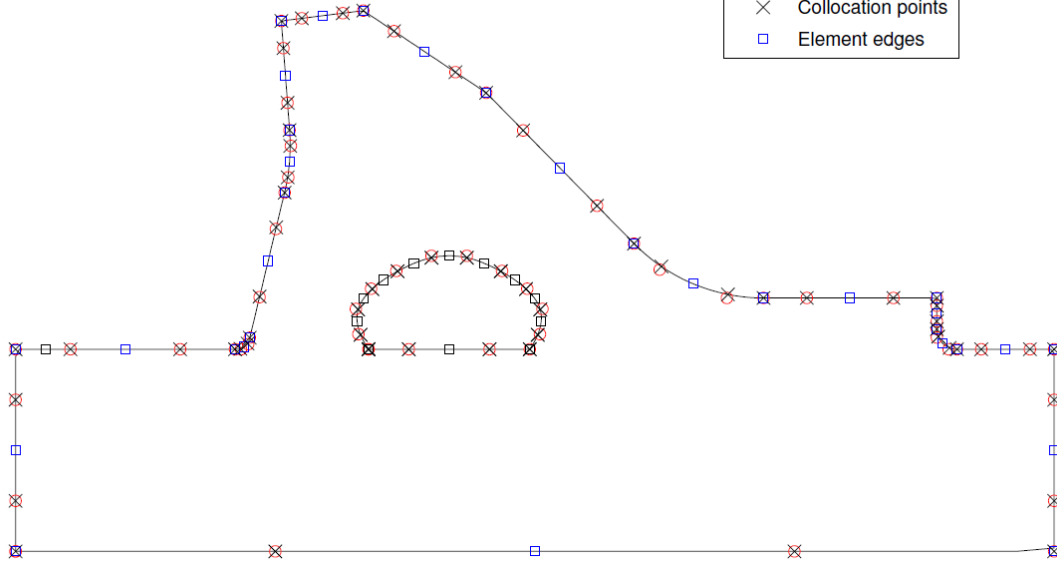
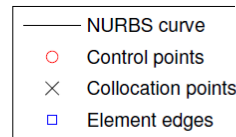
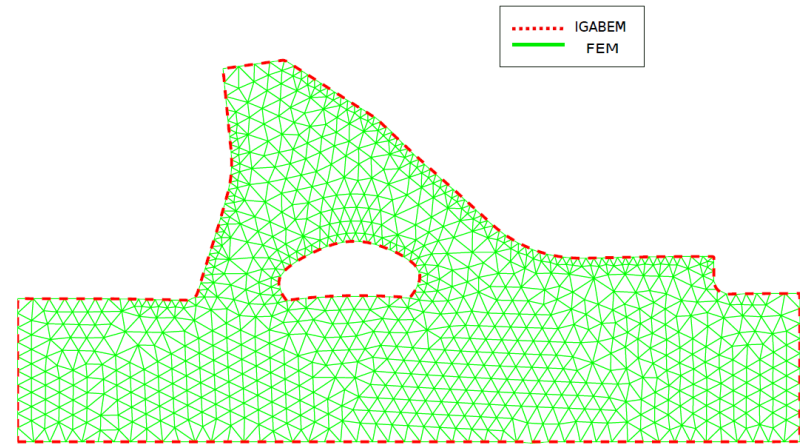
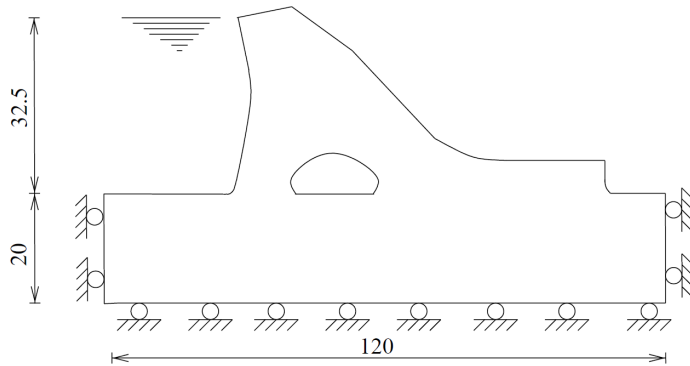


- Exact geometry.
- High order continuity.
- *hpk*-refinement

Nuclear reactor

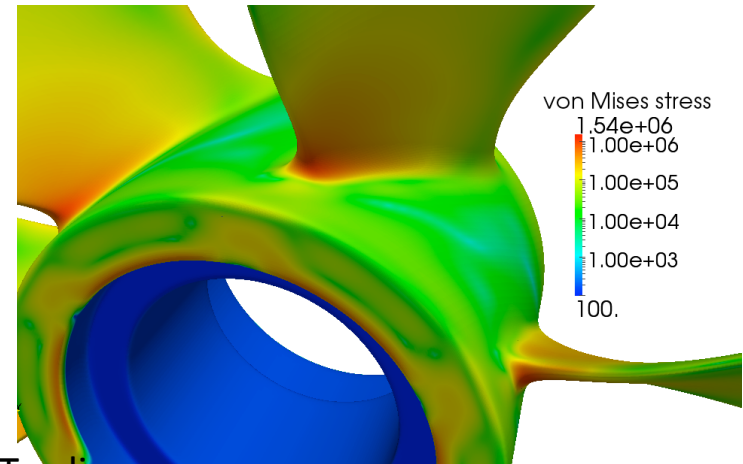
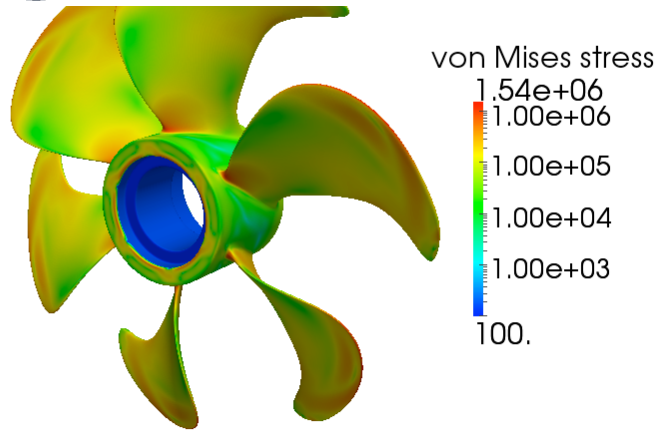
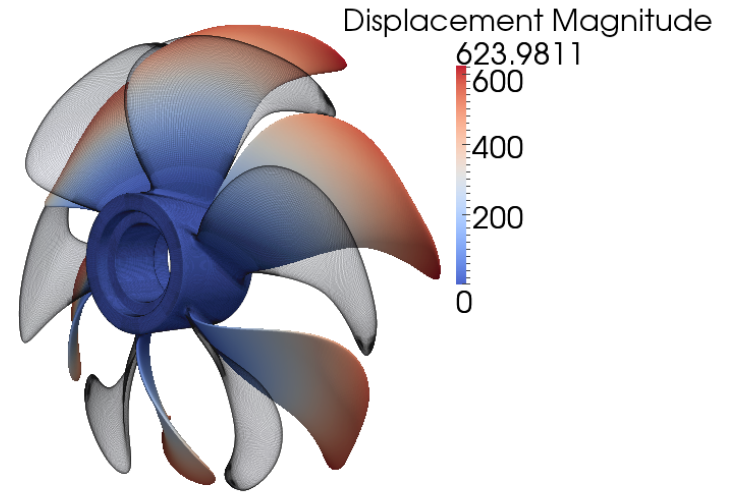
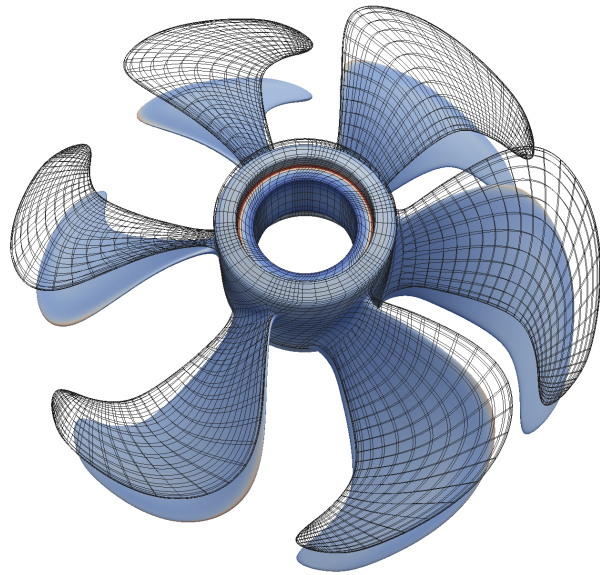


Dam



Stress analysis without meshing: isogeometric boundary-element method
ICE Proceeding, 2013, H Lian, RN Simpson, SPA Bordas

Propeller: NURBS would require several patches - single patch T-splines



Isogeometric boundary element analysis using unstructured T-splines

MA Scott, RN Simpson, JA Evans, S Lipton, SPA Bordas, TJR Hughes, TW Sederberg

CMAME, 2013.

Part I.b.1

Shape optimisation directly from CAD

92

Stéphane P.A. Bordas, Pierre Kerfriden, Elena Atroshchenko, Xuan Peng, Haojie Lian

IGABEM sensitivity analysis formulation

Governing equations in parametric space, which can be viewed as material coordinate system

$$\int_{\Gamma} \mathbf{T}(\mathbf{s}(\zeta), \mathbf{x}(\xi)) [\mathbf{u}(\mathbf{x}(\xi)) - \mathbf{u}(\mathbf{s}(\zeta))] J(\xi) d\xi = \int_{\Gamma} \mathbf{U}(\mathbf{s}(\zeta), \mathbf{x}(\xi)) \mathbf{t}(\mathbf{x}(\xi)) J(\xi) d\xi$$

Differentiate the equation w.r.t. design variables (**implicit differentiation**)

$$\begin{aligned} & \int_{\Gamma} (\mathbf{T}_{,m} J + \mathbf{T} J_{,m}) (\mathbf{u} - \mathbf{u}^s) d\xi + \int_{\Gamma} (\mathbf{T} J) (\mathbf{u}_{,m} - \mathbf{u}_{,m}^s) d\xi \\ &= \int_{\Gamma} (\mathbf{U}_{,m} J + \mathbf{U} J_{,m}) \mathbf{t} d\xi + \int_{\Gamma} (\mathbf{U} J) \mathbf{t}_{,m} d\xi \end{aligned}$$

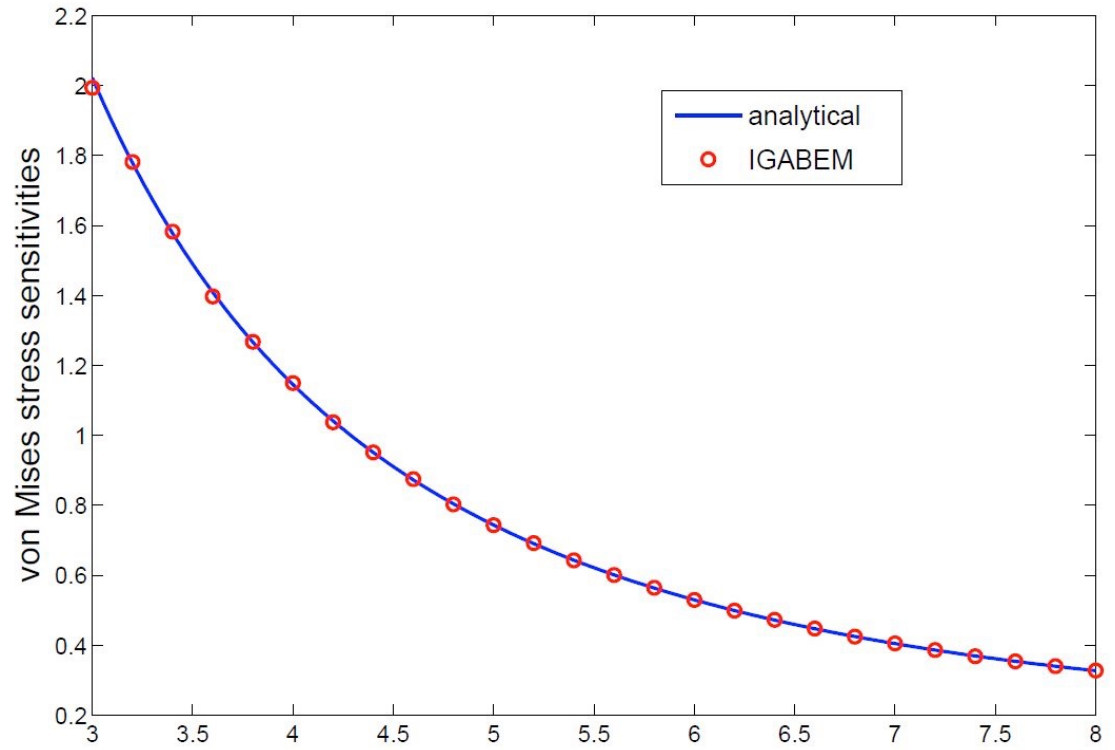
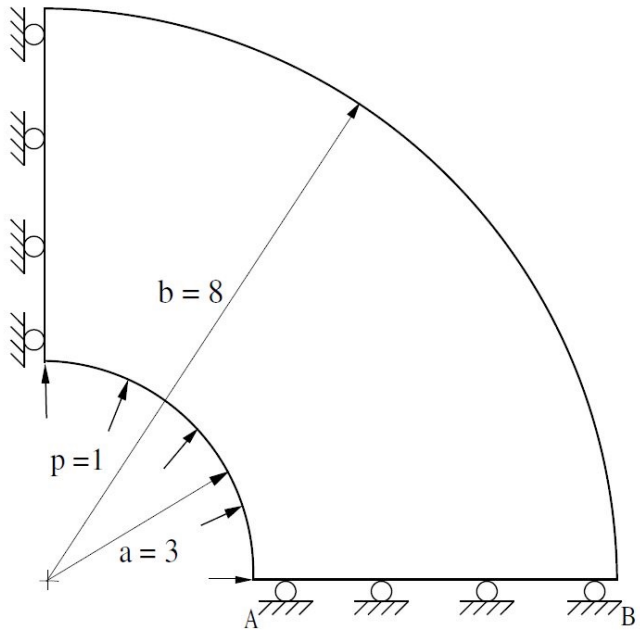
Discretise the derivatives of displacement and traction using NURBS basis

$$\begin{aligned} \mathbf{u}_{,m} &= \sum_{A=1}^{n_A} N_A(\xi) \mathbf{u}_{,m}^A = N_A(\xi) \mathbf{u}_{,m}^A \\ \mathbf{t}_{,m} &= \sum_{B=1}^{n_B} N_B(\xi) \mathbf{t}_{,m}^B = N_B(\xi) \mathbf{t}_{,m}^B \end{aligned}$$

Finally

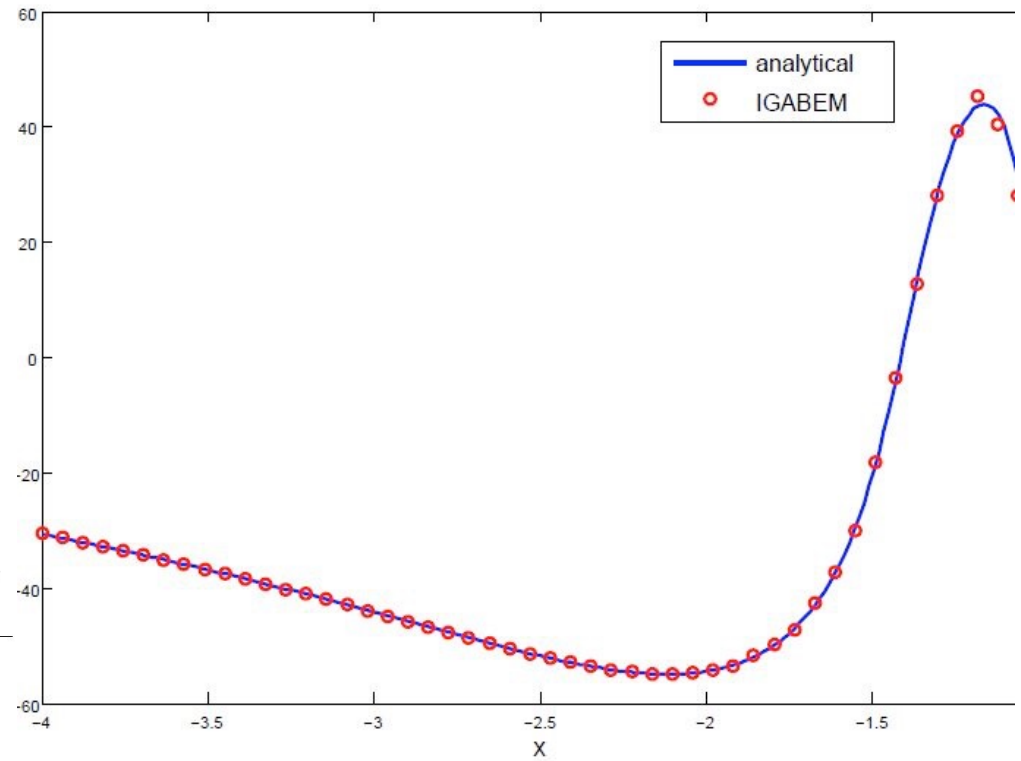
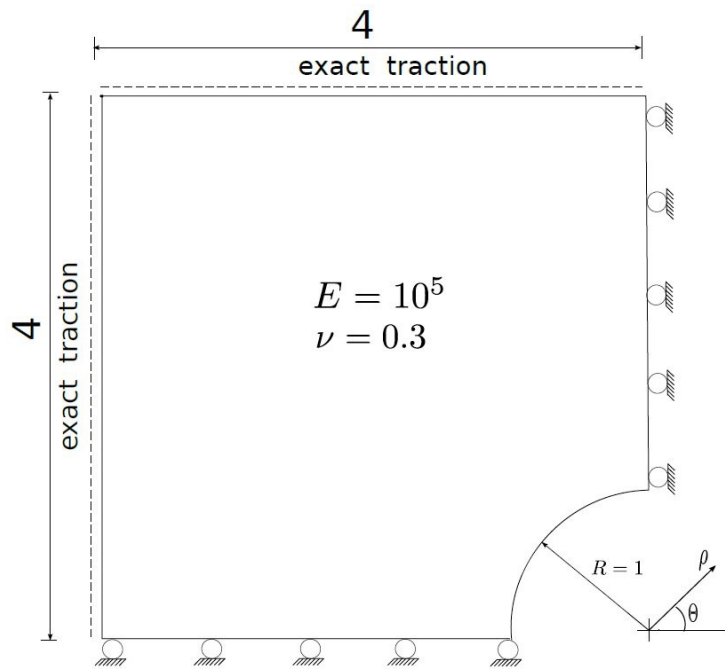
$$\mathbf{H}_m \mathbf{u} + \mathbf{H} \mathbf{u}_m = \mathbf{G}_m \mathbf{t} + \mathbf{G} \mathbf{t}_m$$

Pressure cylinder problem



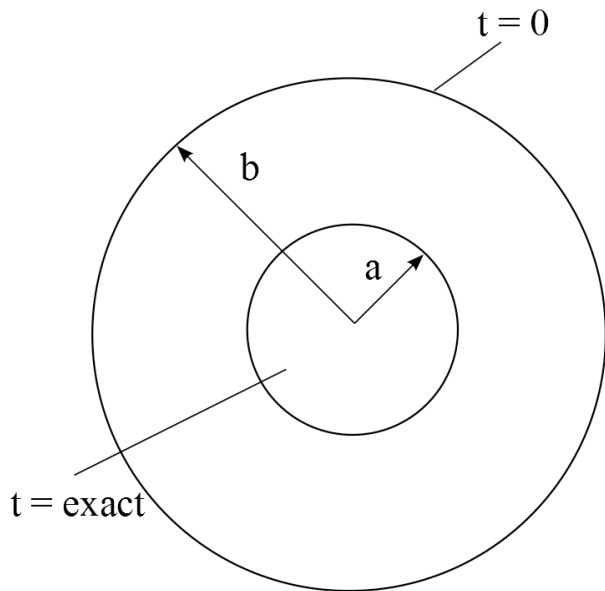
Design variable is outer circle radius b

Infinite plate with a hole

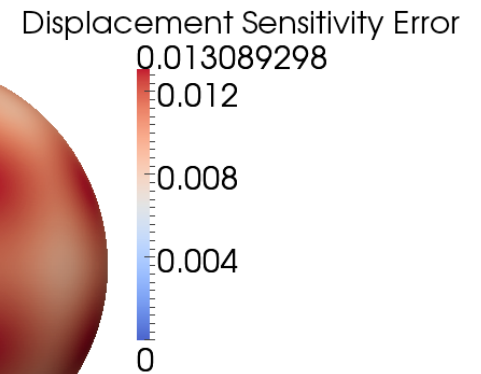
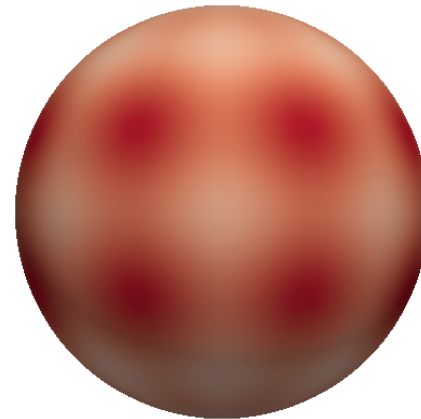
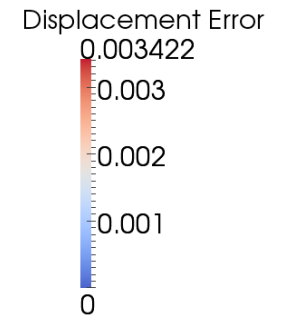
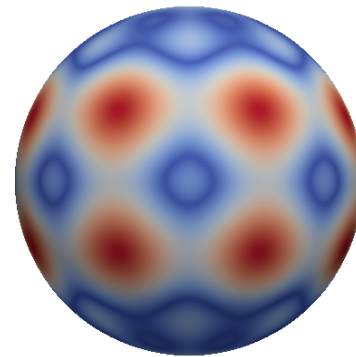


Design variable is radius R

3D Lamé problem

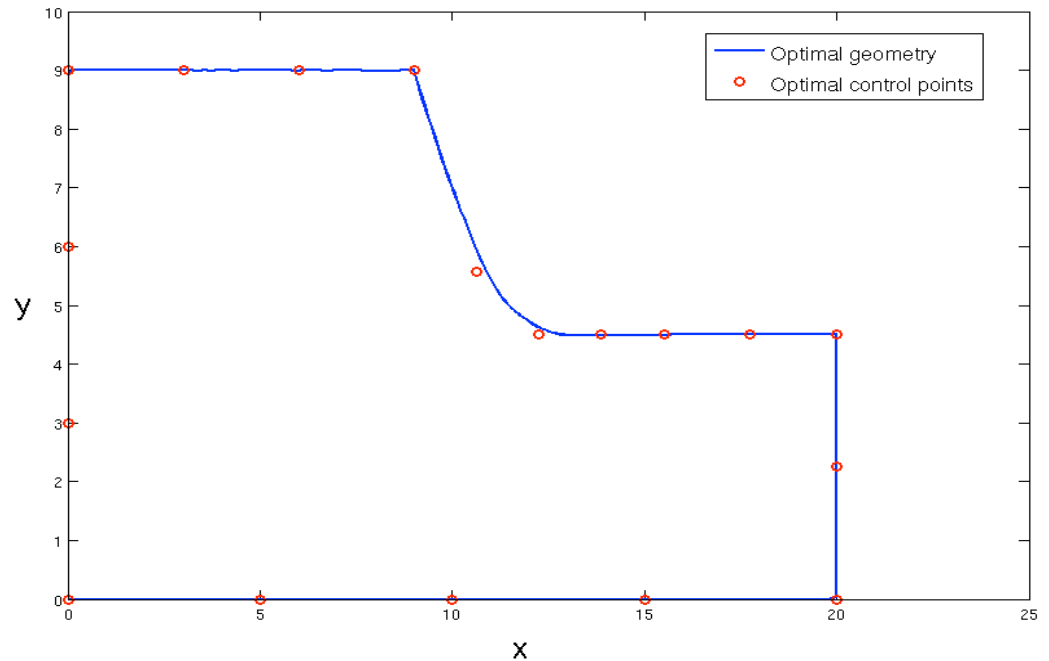
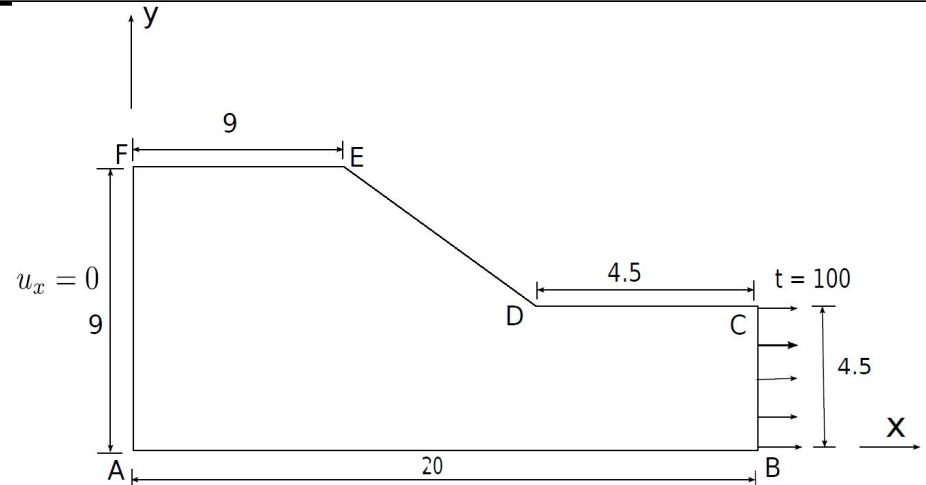


Design parameter: b

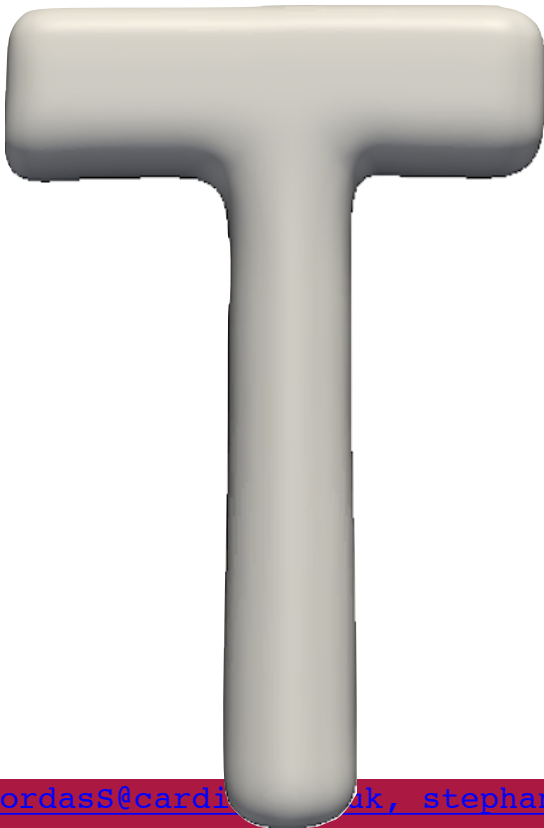


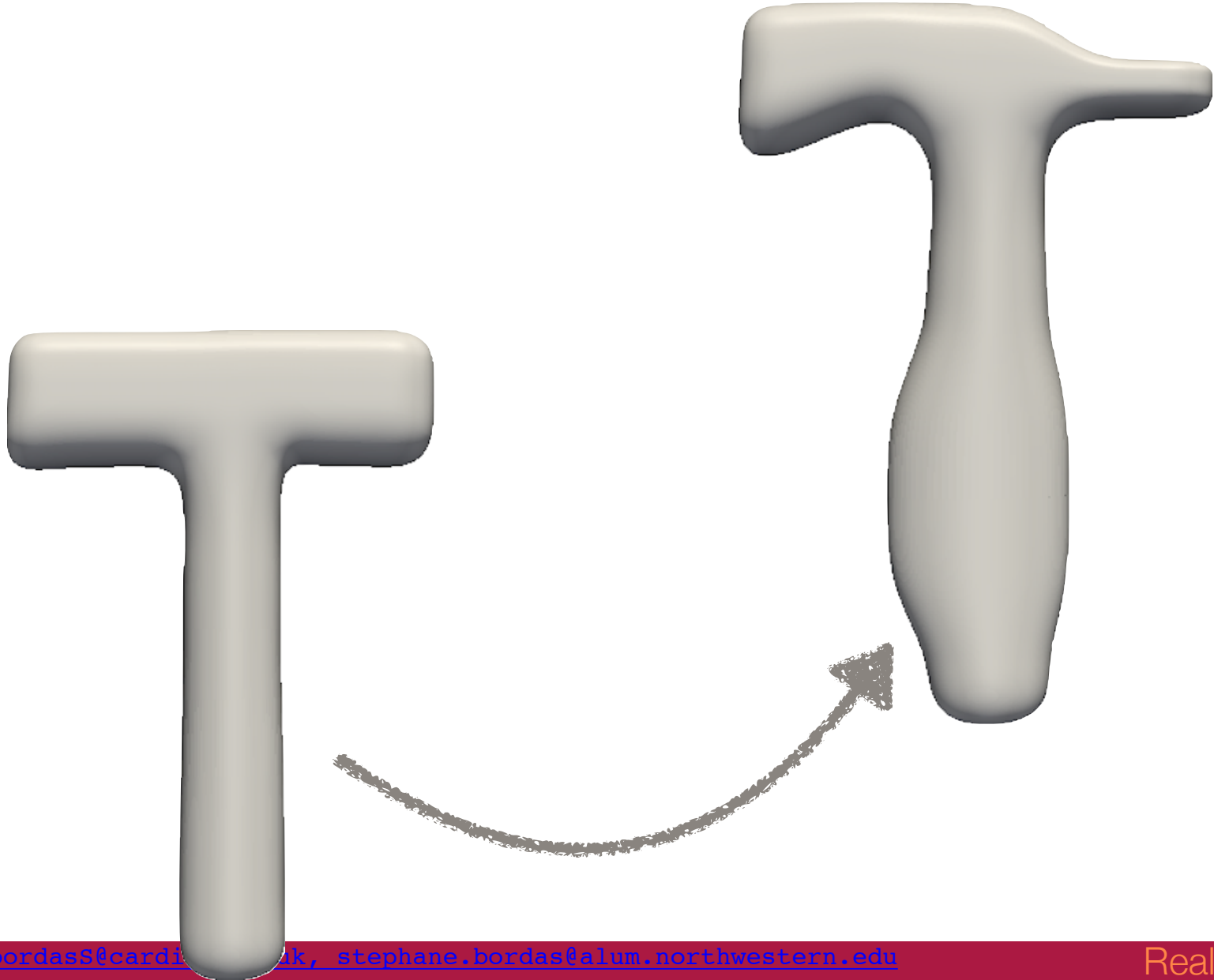
Fillet

Design curve is *ED*.
Minimise the area without violating von Mises stress criterion.



- IGA
- BEM
- T-splines
- Control points and weights as design variables
- Maximize stiffness, minimise volume







R. Alwood, G. Cornes, “A polygonal finite element for plate bending problems using the assumed stress approach”, *International Journal for Numerical Methods in Engineering*, 1(2): 135–149, 1969.

T. Belytschko, Y. Lu, L. Gu, “Element-free Galerkin methods”, *International Journal for Numerical Methods in Engineering*, 37: 229–256, 1994.

T. Belytschko, T. Black, “Elastic crack growth in finite elements with minimal remeshing”, *International Journal for Numerical Methods in Engineering*, 45: 601–620, 1999.

R. Mittal, G. Iaccarino, “Immersed boundary methods”, *Annual Review of Fluid Mechanics*, 37: 239–261, 2005.

G.R. Liu, K. Dai, T. Nguyen, “A smoothed finite element method for mechanics problems”, *Computational Mechanics*, 39: 859–877, 2007.

LB da Veiga, F Brezzi, LD Marini - Virtual Elements for linear elasticity problems *SIAM Journal on Numerical Analysis*, 2013.



F. Rizzo, “An integral equation approach to boundary value problems of classical elastostatics”, *Quart. Appl. Math*, 25(1): 83–95, 1967.

R. Glowinski, T. Pan, J. Periaux, “A fictitious domain method for Dirichlet problem and applications”, *Computer Methods in Applied Mechanics and Engineering*, 111(3-4): 283–303, 1994.

C. Song, J. Wolf, “The scaled boundary finite-element method—alias consistent infinitesimal finite-element cell method—for elastodynamics”, *Computer Methods in Applied Mechanics and Engineering*, 147(3): 329–355, 1997.

R. Simpson, S. Bordas, J. Trevelyan, T. Rabczuk, “A two-dimensional isogeometric boundary element method for elastostatic analysis”, *Computer Methods in Applied Mechanics and Engineering*, 209-212: 87–100, 2012.

Isogeometric boundary element analysis using unstructured T-splines
MA Scott, RN Simpson, JA Evans, S Lipton, SPA Bordas, TJR Hughes, TW Sederberg
Computer Methods in Applied Mechanics and Engineering, 2013.



E. Saiki, S. Biringen, “Numerical simulation of a cylinder in uniform flow: application of a virtual boundary method”, *Journal of Computational Physics*, 123(2): 450–465, 1996.

H. Johansen, P. Colella, “A Cartesian grid embedded boundary method for Poisson’s equation on irregular domains”, *Journal of Computational Physics*, 147(1): 60–85, 1998.

T. Ye, R. Mittal, H. Udaykumar, W. Shyy, “An accurate Cartesian grid method for viscous incompressible flows with complex immersed boundaries”, *Journal of Computational Physics*, 156(2): 209–240, 1999.

M. Moumnassi, S. Belouettar, E. Bechet, S. Bordas, D. Quoirin, M. Potier Ferry, “Finite element analysis on implicitly defined domains: An accurate representation based on arbitrary parametric surfaces”, *Computer Methods in Applied Mechanics and Engineering*, 200(5): 774–796, 2011.

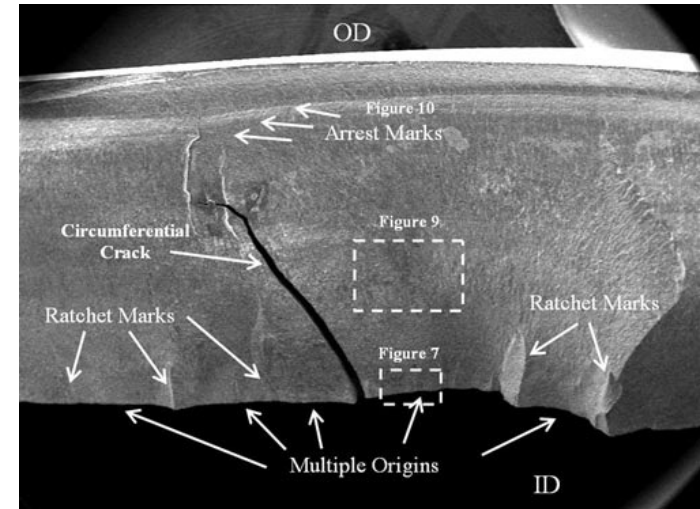
Part I.b.2 Isogeometric Boundary Element Method for Damage Tolerance Assessment directly from CAD

➤ Fatigue Fracture Failure of Structure

- Initiation: micro defects
- Loading : cyclic stress state (temperature, corrosion)

➤ Numerical methods for crack growth

- Volume methods:
FEM, XFEM/GFEM, Meshfree
- Boundary methods: BEM

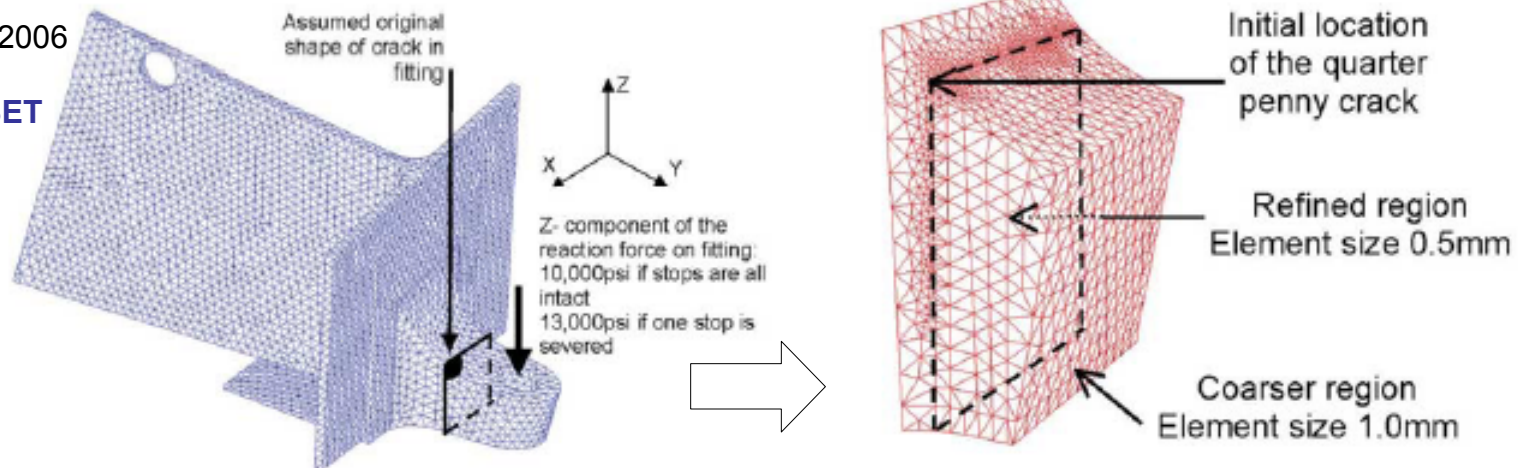


Fatigue cracking of nozzle sleeve

<http://met-tech.com/>

Bordas & Moran, 2006

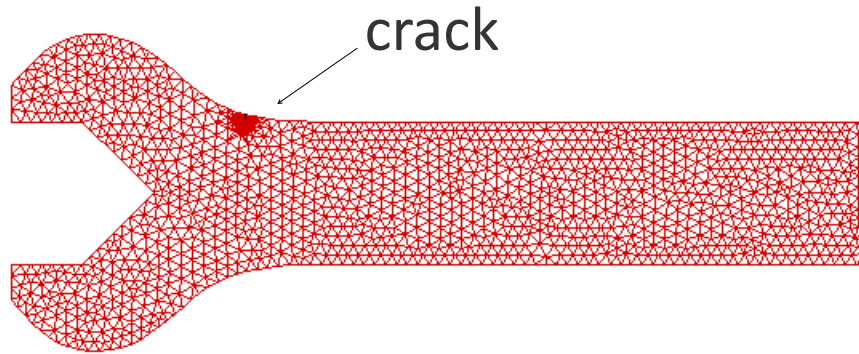
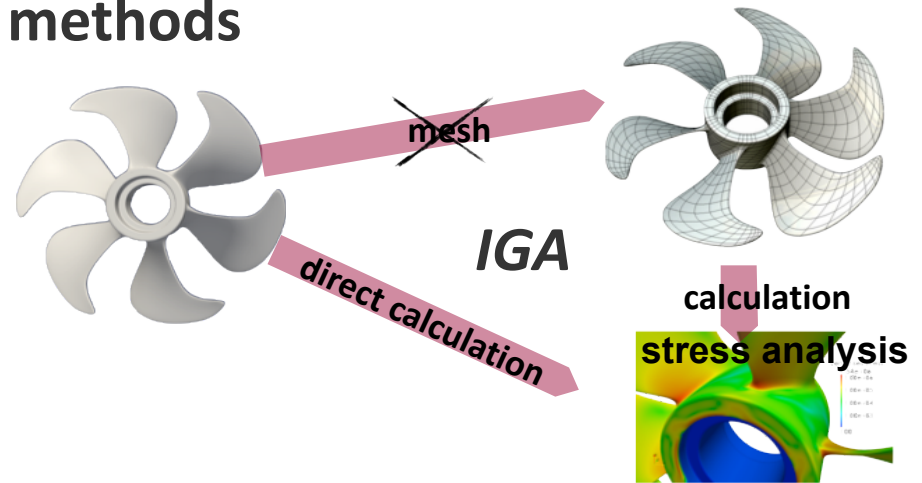
XFEM+LEVEL SET



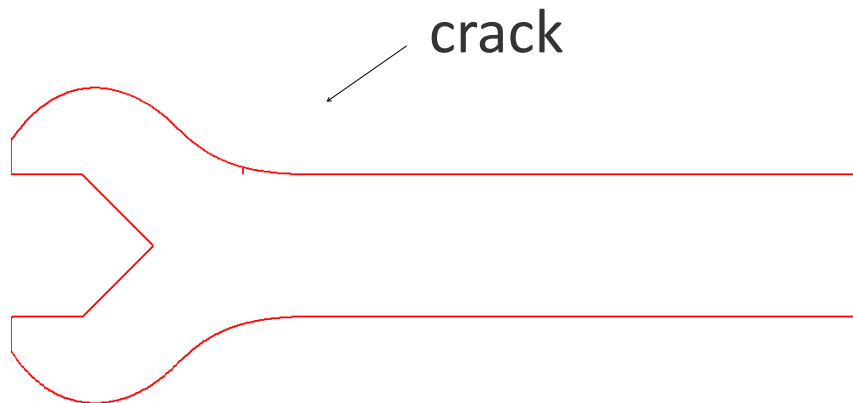
➤ Challenges in volume-based methods

- Remeshing (FEM)
- Local mesh refinement

Efficiency & Accuracy



XFEM
adaptive refinement



IGABEM
Direct CAD used

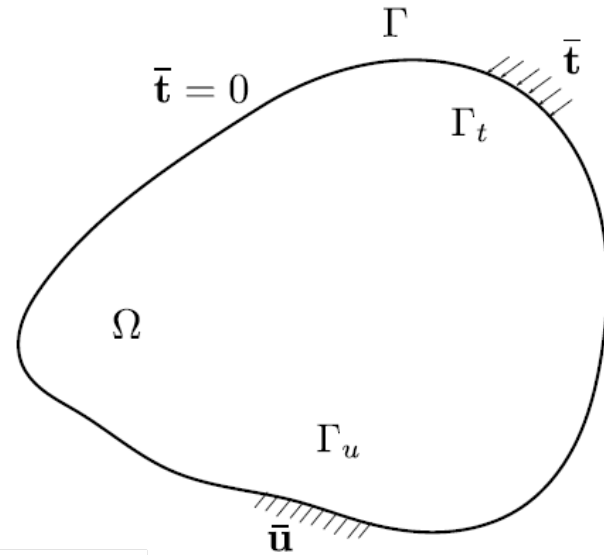
Weighted residual method, collocation

Linear elasticity problem:

$$\begin{aligned}\mathcal{L}(\mathbf{u}) &= \nabla \cdot (\mathbf{C}\nabla^s \mathbf{u}) = \mathbf{f}, & \text{in } \Omega \\ \mathbf{u} &= \bar{\mathbf{u}}, & \text{on } \Gamma_u \\ \mathbf{t} &= (\mathbf{C}\nabla^s \mathbf{u}) \cdot \mathbf{n} = \bar{\mathbf{t}}, & \text{on } \Gamma_t\end{aligned}$$

Approximation of \mathbf{u} :

$$\mathbf{u}^h = \bar{\mathbf{u}} + \sum_{I=1}^n N_I(\mathbf{x}) \mathbf{u}^I$$



Weighted residual form:

$$\int_{\Omega} (\nabla \cdot (\mathbf{C}\nabla^s \mathbf{u}) - \mathbf{f}) \cdot \mathbf{v} d\Omega + \int_{\Gamma_t} (\mathbf{t} - \bar{\mathbf{t}}) \cdot \mathbf{v} d\Gamma = 0$$

Collocation method:

$$\mathbf{v}(\mathbf{z}) = \sum_{I=1}^k \mathbf{v}^I \delta(\mathbf{s}_I, \mathbf{z})$$

sifting property:

$$\int_{\Omega} g(\mathbf{z}) \delta(\mathbf{s}, \mathbf{z}) d\Omega = g(\mathbf{s})$$

Galerkin method (variational principle):

$$\mathbf{v}(\mathbf{z}) = \sum_{I=1}^k N_I(\mathbf{z}) \mathbf{v}^I$$

$$\int_{\Omega} (\nabla \mathbf{v} : \mathbf{C}\nabla^s \mathbf{u} - \mathbf{f} \cdot \mathbf{v}) d\Omega + \int_{\Gamma_t} \mathbf{t} \cdot \mathbf{v} d\Gamma = 0$$

Kelvin fundamental solution

Navier equation: $\mu \nabla^2 \mathbf{u} + (\mu + \lambda) \nabla(\nabla \cdot \mathbf{u}) = \mathbf{f}$

Kelvin solution: assuming a unit concentrated force applied on a point \mathbf{s} in the infinite domain $\mathbf{f}(\mathbf{z}) = \mathbf{e} \delta(\mathbf{s}, \mathbf{z})$, we seek $\mathbf{u}(\mathbf{z})$ and $\mathbf{t}(\mathbf{z})$ for any point \mathbf{z}

$$u_i^* = U_{ij} e_j \quad t_i^* = T_{ij} e_j$$

for 3D problems, the expressions are:

$$U_{ij}(\mathbf{s}, \mathbf{z}) = \frac{1}{16\pi\mu(1-\nu)r} [(3-4\nu)\delta_{ij} + r_{,i}r_{,j}]$$

$$T_{ij}(\mathbf{s}, \mathbf{z}) = -\frac{1}{8\pi(1-\nu)} \left[\frac{\partial r}{\partial n} ((1-2\nu)\delta_{ij} + 3r_{,i}r_{,j}) - (1-2\nu)(n_j r_{,i} - n_i r_{,j}) \right]$$

Boundary integral equations (BIEs) and IGABEM crack modeling

• **Displacement BIE**
$$c_{ij}(\mathbf{s})u_j(\mathbf{s}) + \oint_{\Gamma} T_{ij}(\mathbf{s}, \mathbf{x})u_j(\mathbf{x})d\Gamma(\mathbf{x}) = \int_{\Gamma} U_{ij}(\mathbf{s}, \mathbf{x})t_j(\mathbf{x})d\Gamma(\mathbf{x})$$

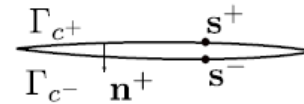
• **Traction BIE**
$$c_{ij}(\mathbf{s})t_j(\mathbf{s}) + \oint_{\Gamma} S_{ij}(\mathbf{s}, \mathbf{x})u_j(\mathbf{x})d\Gamma(\mathbf{x}) = \int_{\Gamma} K_{ij}(\mathbf{s}, \mathbf{x})t_j(\mathbf{x})d\Gamma(\mathbf{x})$$

• **NURBS approximation**

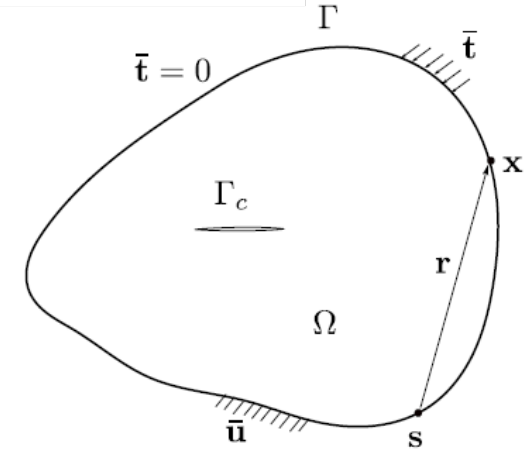
$$u_i(\xi) = \sum_{A=1}^n R_{A,p}(\xi)d_i^A$$

$$t_i(\xi) = \sum_{A=1}^n R_{A,p}(\xi)q_i^A$$

displacement BIE for \mathbf{s}^+

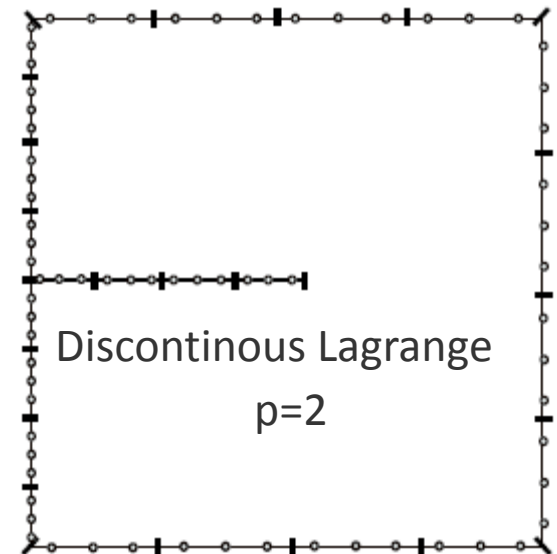
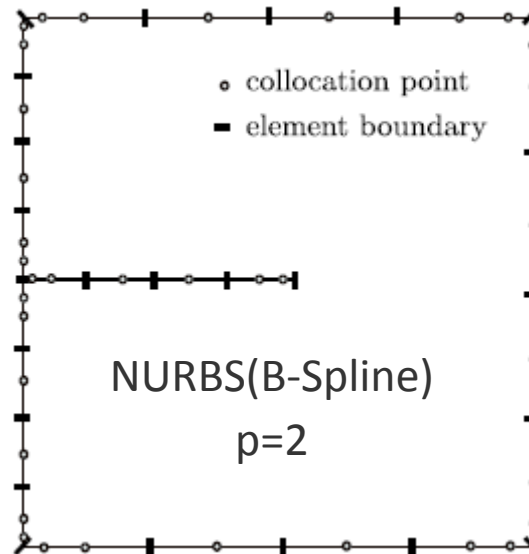


traction BIE for \mathbf{s}^-



• **Collocation: Greville Abcissae**

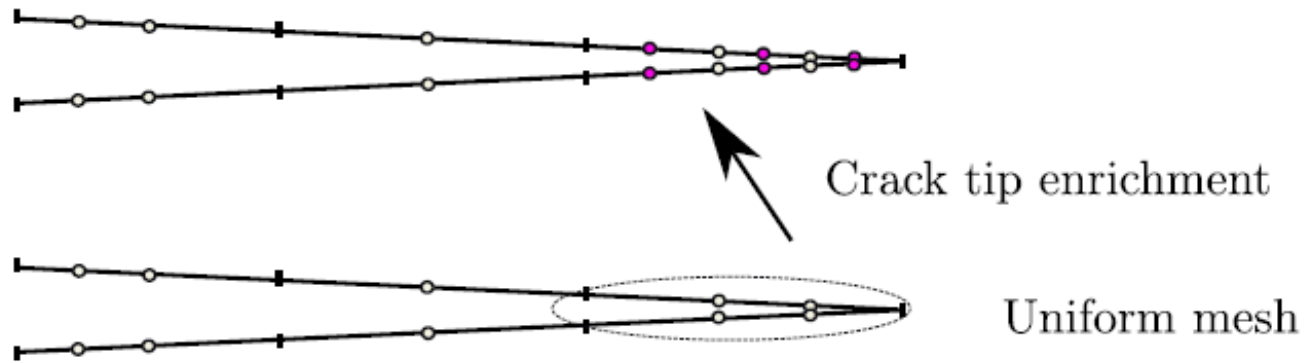
$$\xi_s = \frac{\xi_{i+1} + \dots + \xi_{i+p}}{p}$$



Treatment of crack tip singularity

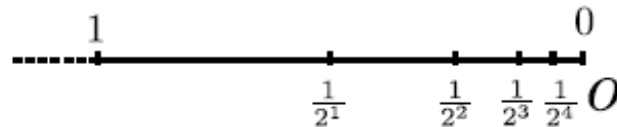
- Partition of unity enrichment (2D)

$$u_i(\mathbf{x}) = \sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) d_i^I + \sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) \phi(\mathbf{x}) a_i^J \quad \phi = \sqrt{r}$$



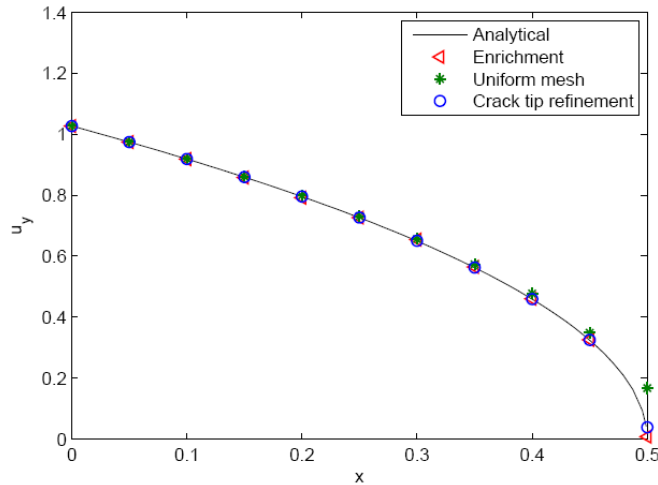
- Original collocation point
- Additional collocation point

Crack tip mesh refinement

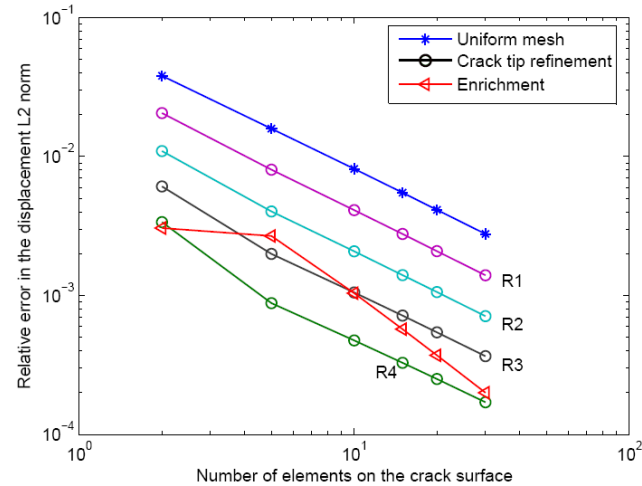


- Consecutive knot insertion at crack tip (2D) or along crack front (3D)

Crack tip refinement VS enrichment

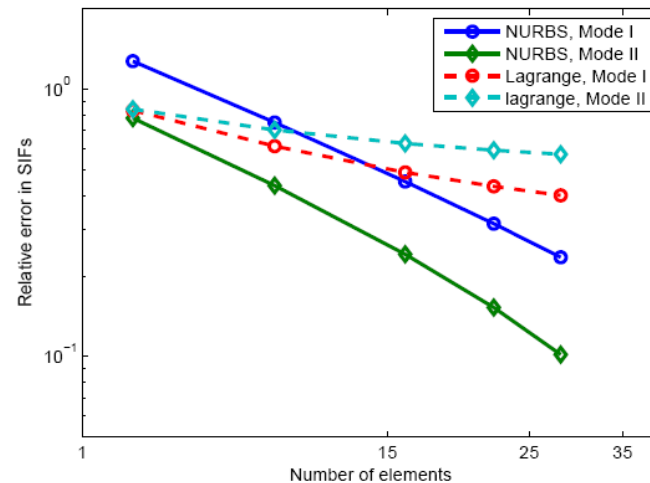
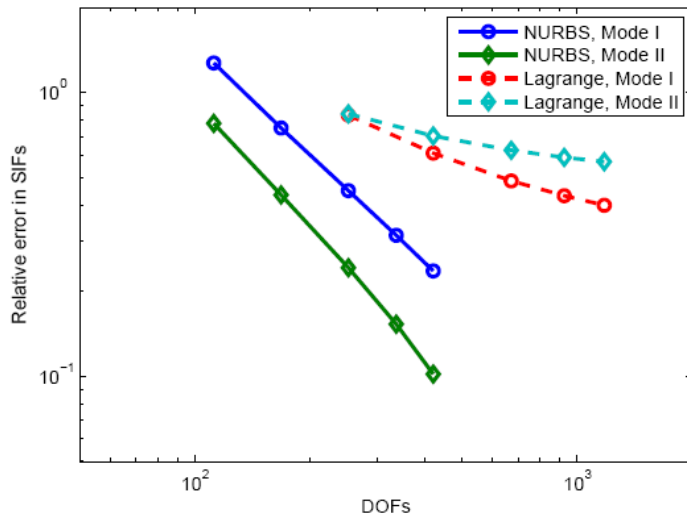


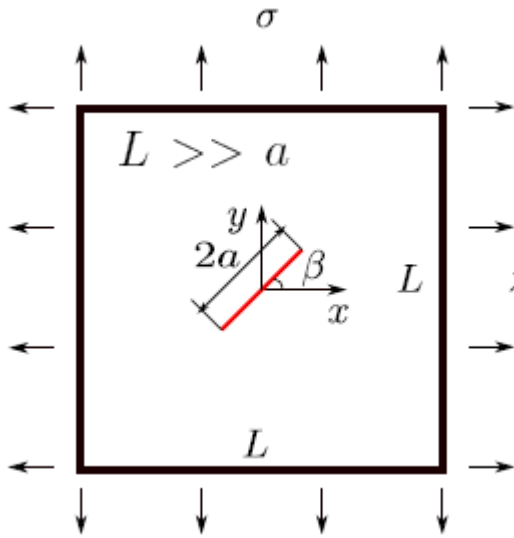
Crack opening displacement



Error in displacement L2 norm

NURBS VS Lagrange: convergence in SIFs, no crack tip treatment





$$K_I = \sigma \sqrt{\pi a} (\cos^2 \beta + \lambda \sin^2 \beta)$$

$$K_{II} = \sigma \sqrt{\pi a} (1 - \lambda) \cos \beta \sin \beta$$

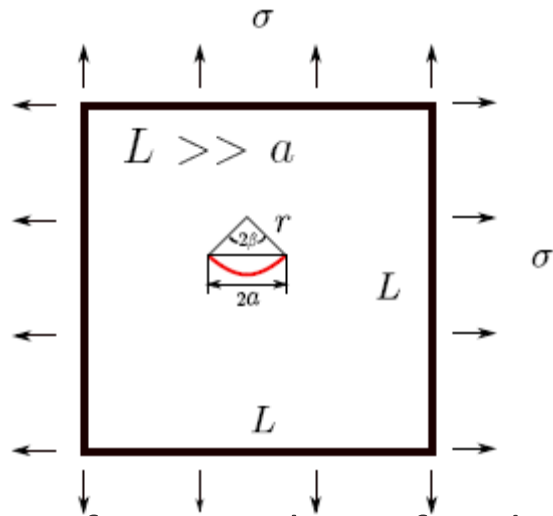
$$\beta = \pi/6, \quad \sigma = 1, \quad \lambda = 0.5$$

- IGABEM(r) : Uniform mesh (refined tip element)
- LBEM: discontinuous Lagrange BEM
- SGBEM: symmetric Galerkin BEM, Sutrahara & Paulino (2004)

m: number of elements in uniform mesh along the crack surface

<i>m</i>	K_I / K_I^{exact}			
	SGBEM	LBEM	IGABEM	IGABEM(r)
3	0.9913	1.00451	1.00982	1.00120
4	1.0002	1.00333	1.00769	1.00105
5	1.0001	1.00268	1.00633	1.00090
6	1.0002	1.00230	1.00539	1.00080
7	1.0003	1.00206	1.00474	1.00074
8	1.0003	1.00190	1.00426	1.00070
9	1.0003	1.00177	1.00389	1.00066
10	1.0003	1.00167	1.00359	1.00064
11	1.0003	1.00159	1.00336	1.00062
12	1.0003	1.00152	1.00316	1.00060
14	1.0003	1.00142	1.00285	1.00058

<i>m</i>	K_{II} / K_{II}^{exact}			
	SGBEM	LBEM	IGABEM	IGABEM(r)
3	1.0075	1.00104	1.00647	1.00146
4	1.0009	1.00129	1.00656	1.00129
5	1.0010	1.00158	1.00607	1.00113
6	1.0009	1.00160	1.00550	1.00102
7	1.0014	1.00153	1.00500	1.00096
8	1.0005	1.00143	1.00458	1.00091
9	0.9997	1.00134	1.00424	1.00087
10	1.0009	1.00126	1.00396	1.00085
11	0.9992	1.00119	1.00373	1.00083
12	1.0013	1.00112	1.00353	1.00081
14	1.0004	1.00102	1.00322	1.00079



$$K_I = \sigma \sqrt{\pi a} \frac{\cos(\beta/2)}{1 + \sin^2(\beta/2)}$$

$$K_{II} = \sigma \sqrt{\pi a} \frac{\sin(\beta/2)}{1 + \sin^2(\beta/2)}$$

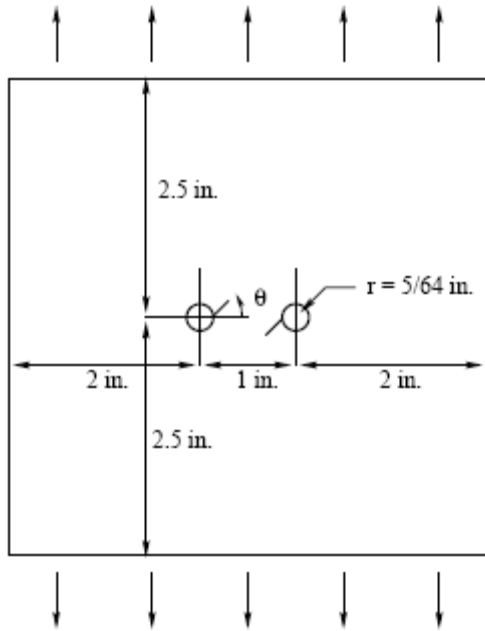
$$\sigma = 1, \quad \beta = \pi/4$$

• Uniform mesh + refined tip element

• Splitting parameter in **J** integral: $r_{split} = 0.03R_J, 0.04R_J, 0.05R_J, 0.06R_J, 0.07R_J$

m : number of elements in uniform mesh along the crack surface

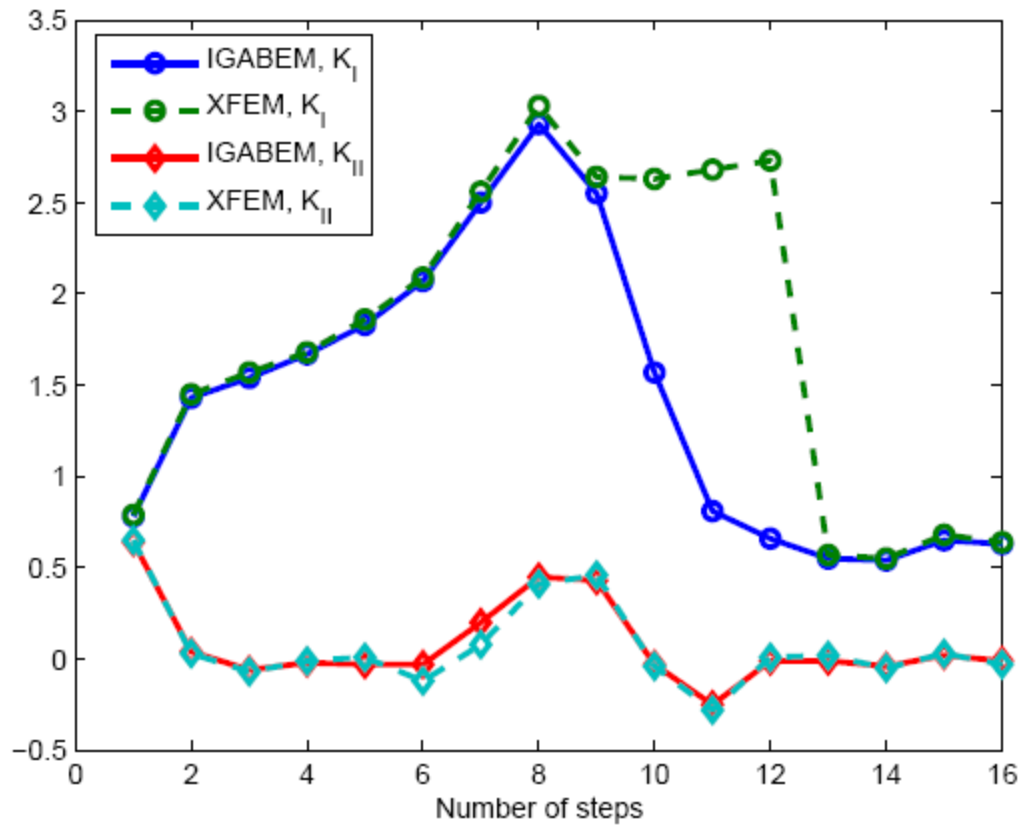
m	K_I/K_I^{exact}		K_{II}/K_{II}^{exact}	
	M integral	J_k integral	M integral	J_k integral
10	1.00045	0.99972	0.97506	1.00309
14	1.00014	0.99979	0.98621	1.00248
17	1.00011	0.99982	0.98642	1.00217
20	1.00009	0.99985	0.98657	1.00195
23	1.00002	0.99987	0.99407	1.00176
26	1.00002	0.99989	0.99413	1.00163

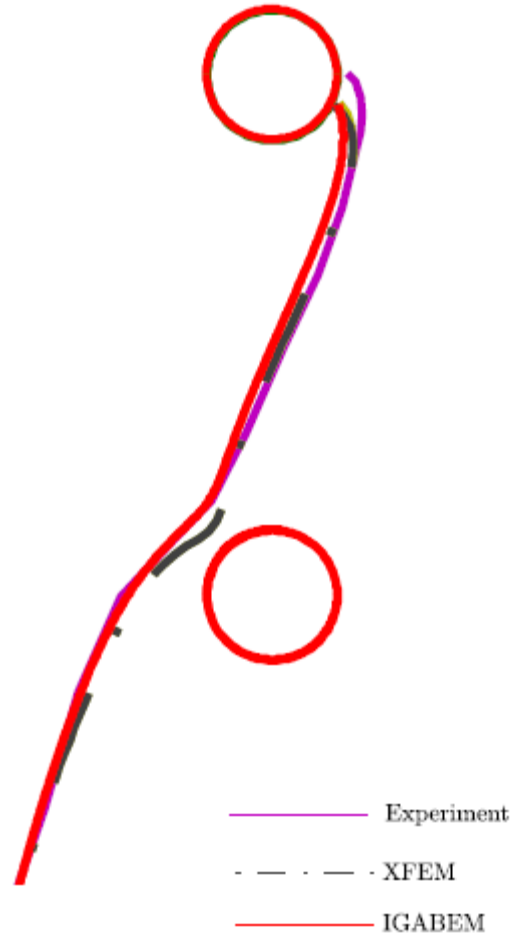
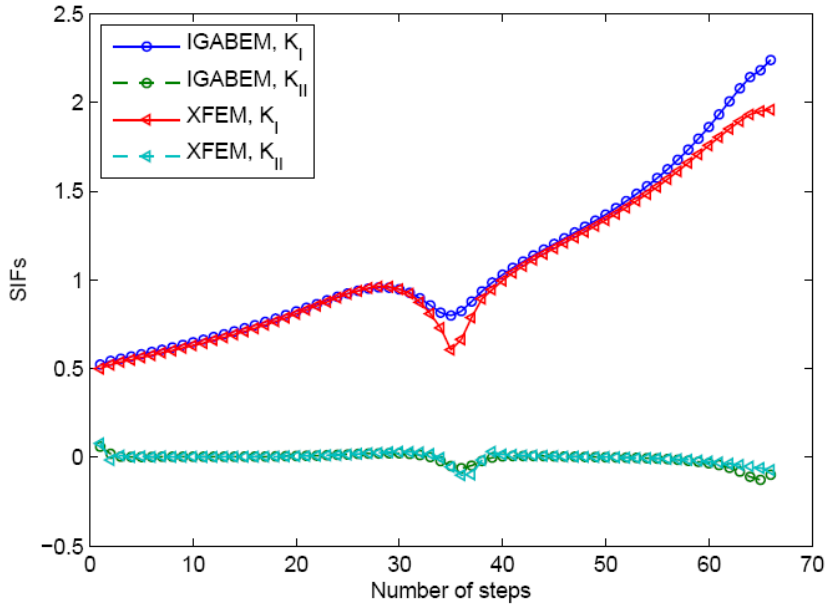
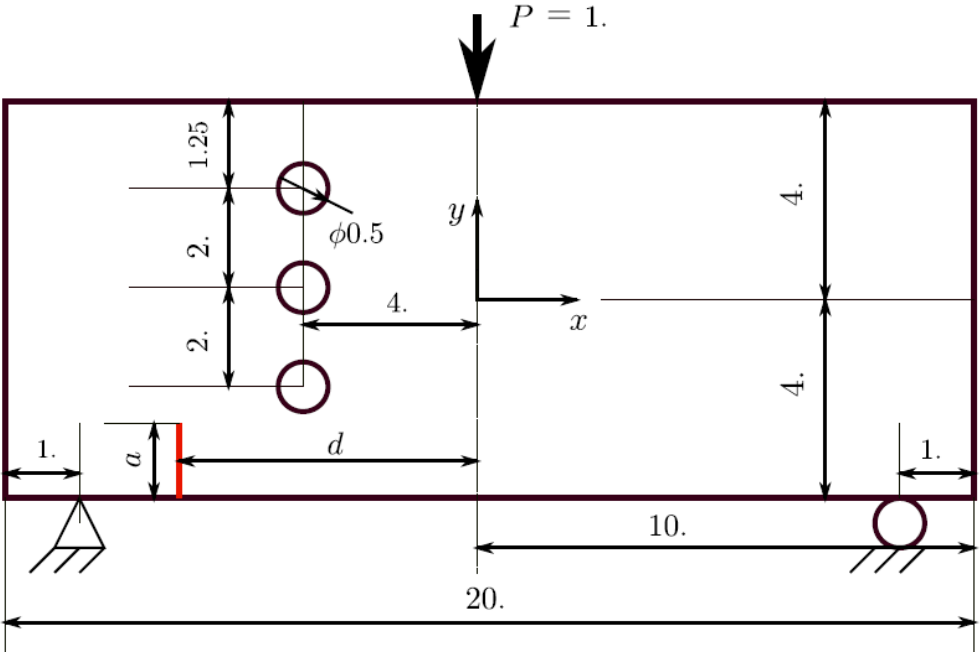


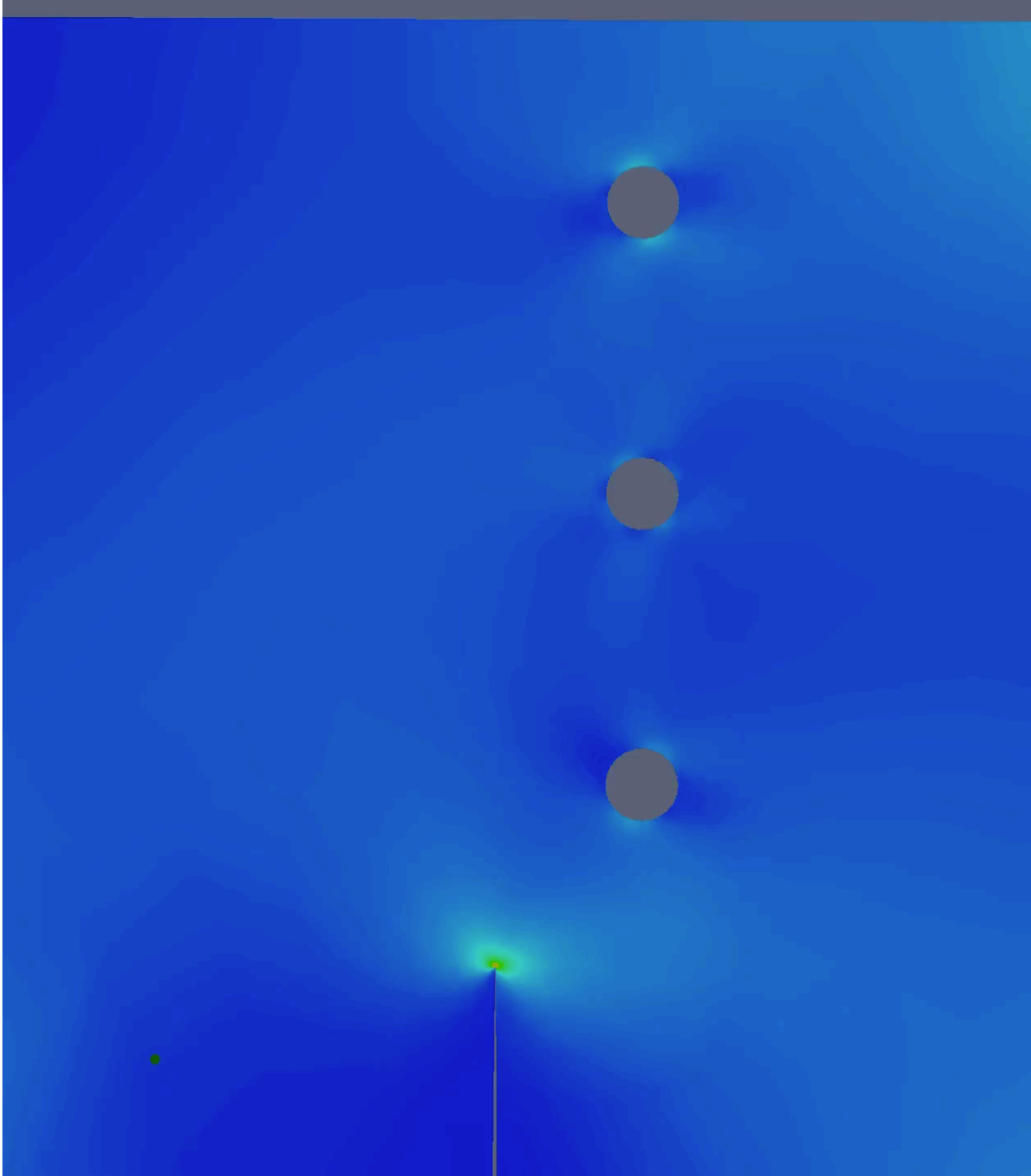
(a) XFEM by Möes et al (1999)



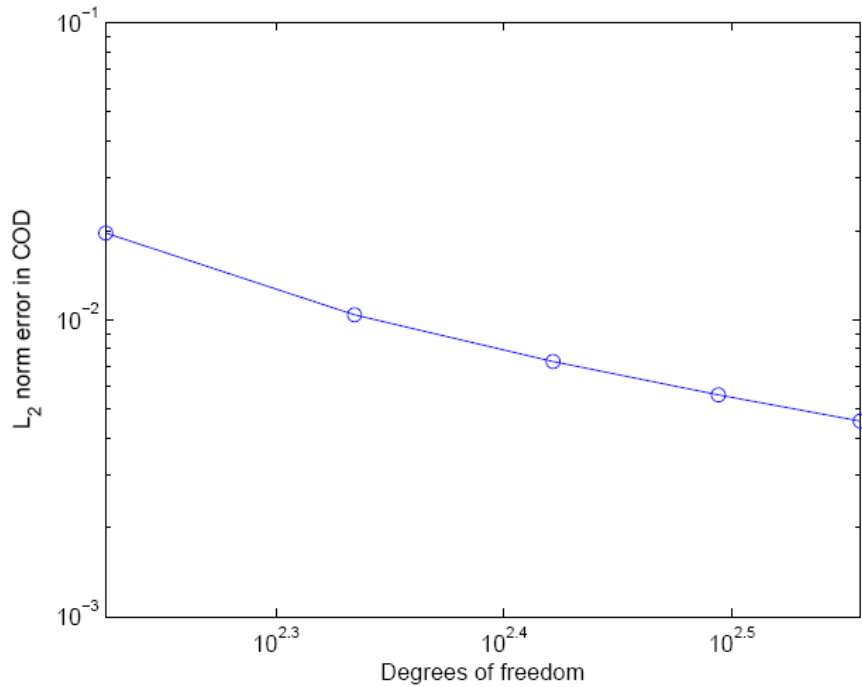
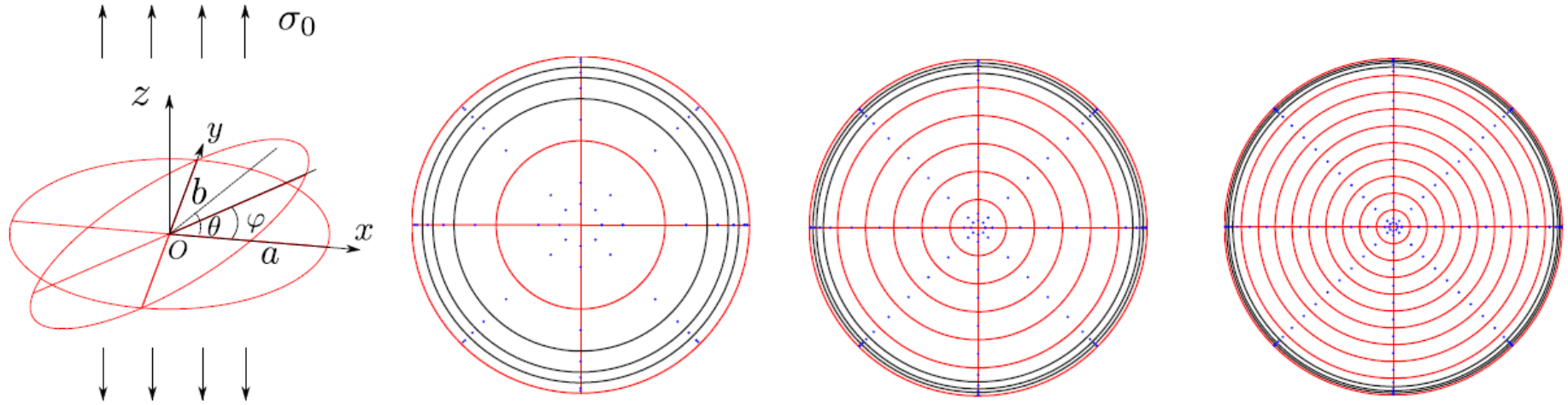
(b) IGABEM



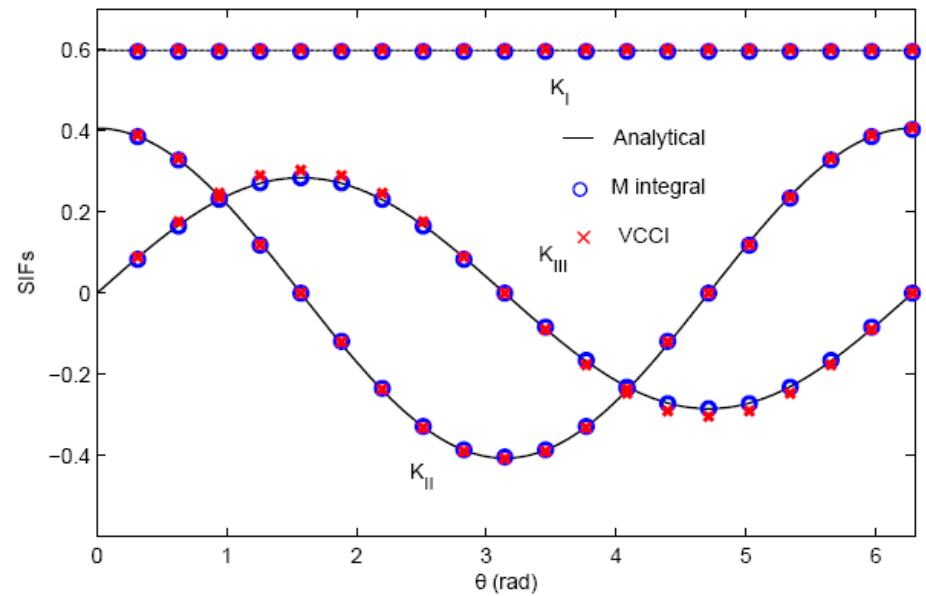




Penny-shaped crack under remote tension



L_2 norm error of COD for penny-shaped crack



stress intensity factors for penny crack with $\varphi = \pi/6$

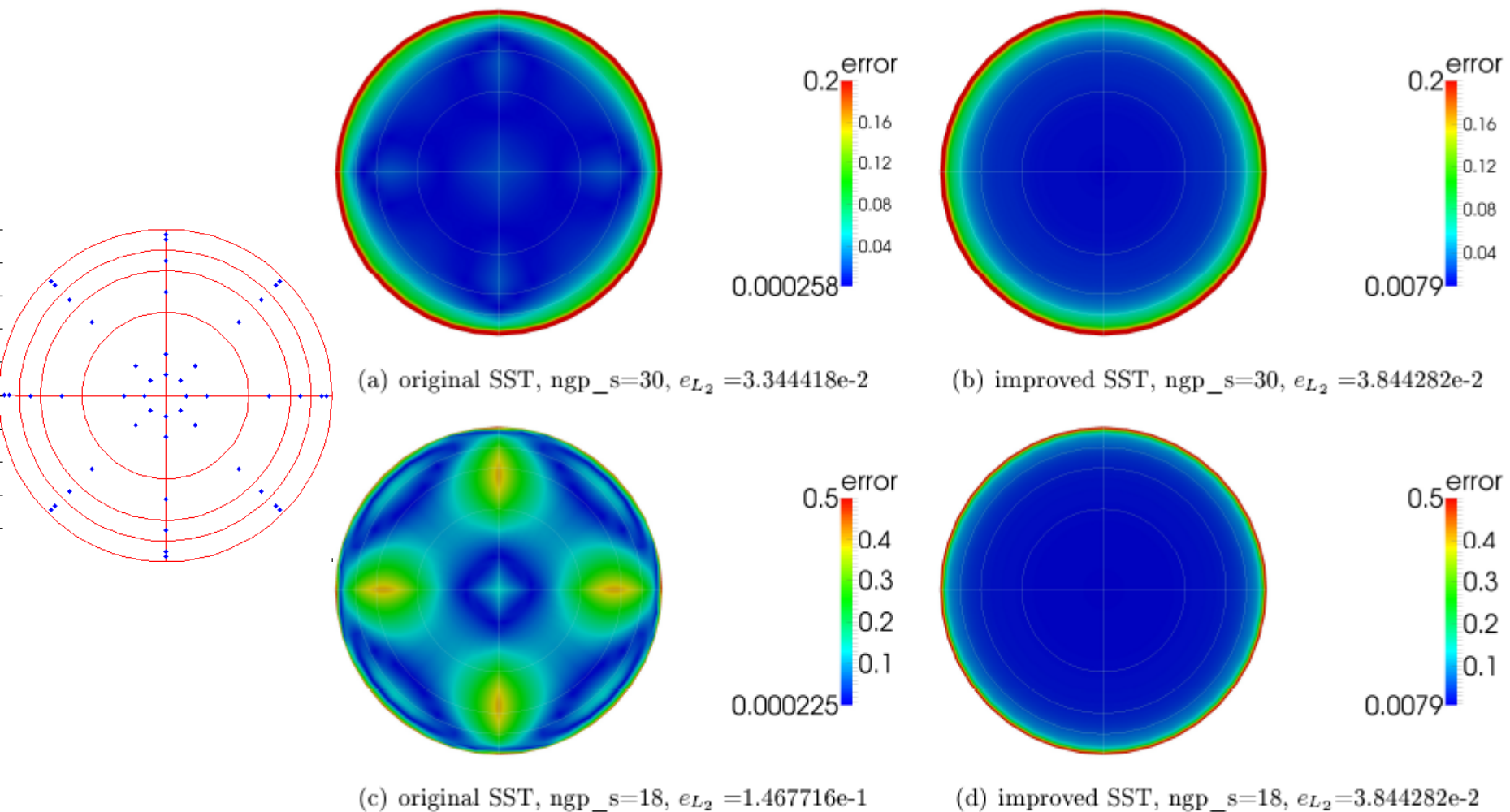
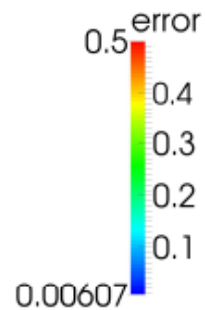
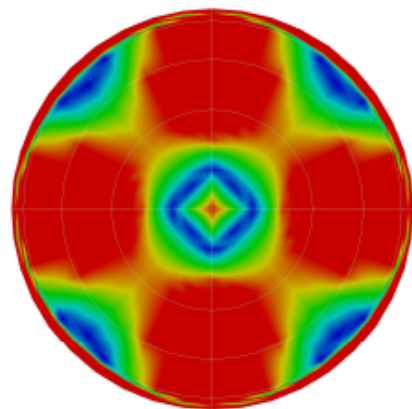
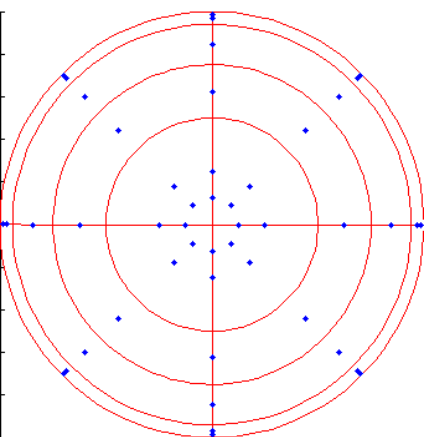
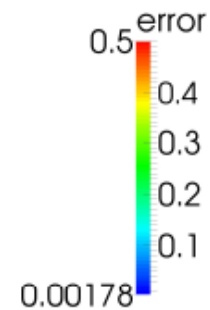
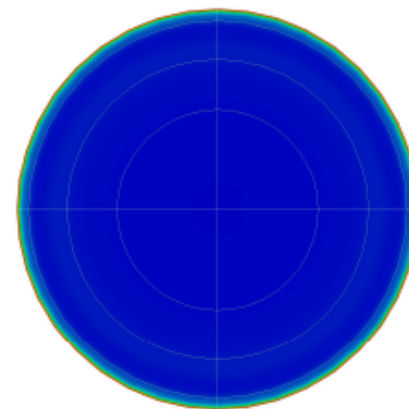


Figure 5: Error in crack opening displacement for penny crack

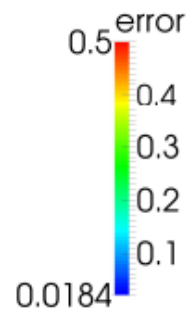
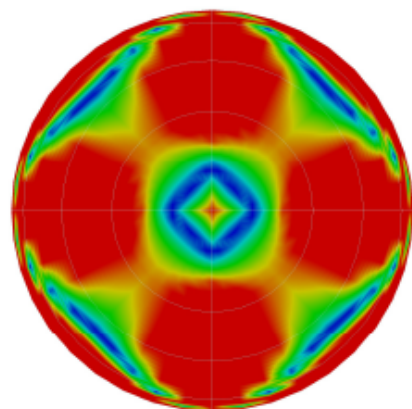
Penny crack under remote tension (embedded crack)



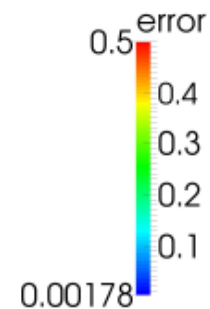
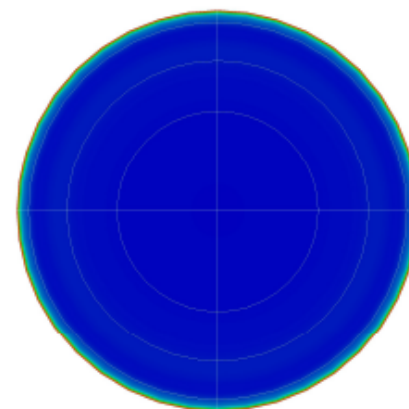
(a) original SST, $ngp_s=30$, $e_{L_2}=8.138911e-1$



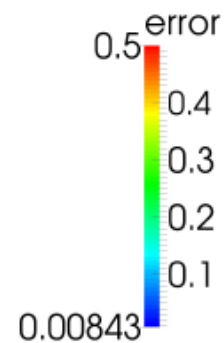
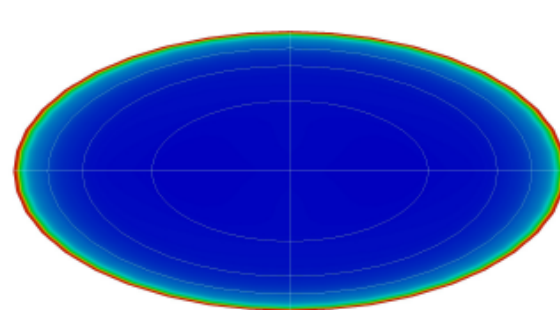
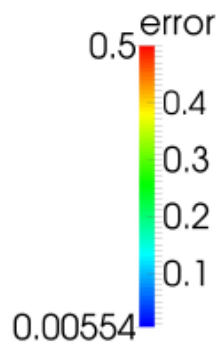
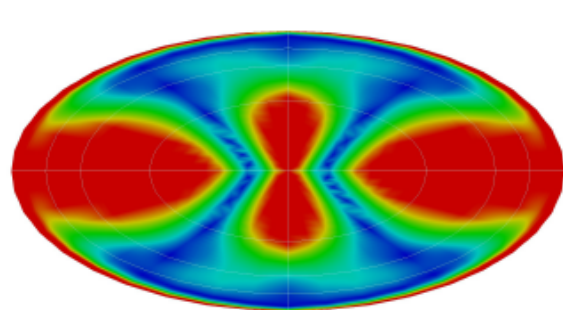
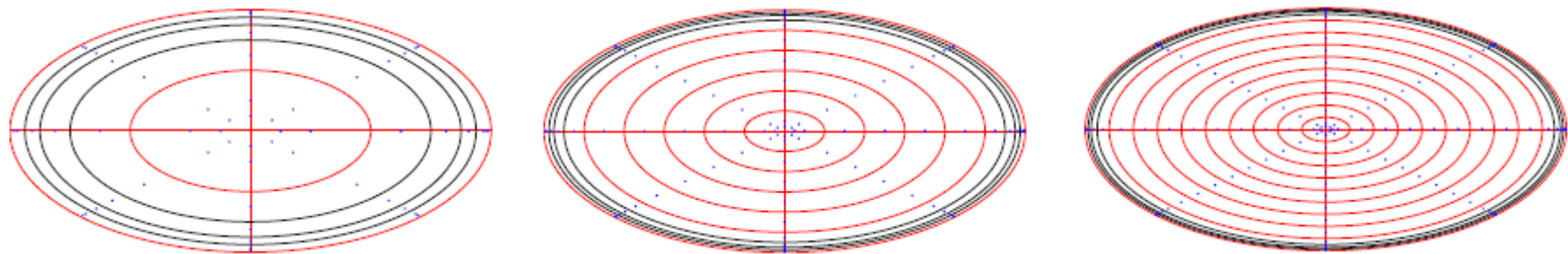
(b) improved SST, $ngp_s=30$, $e_{L_2}=1.755681e-2$



(c) original SST, $ngp_s=18$, $e_{L_2}=7.110011e-1$

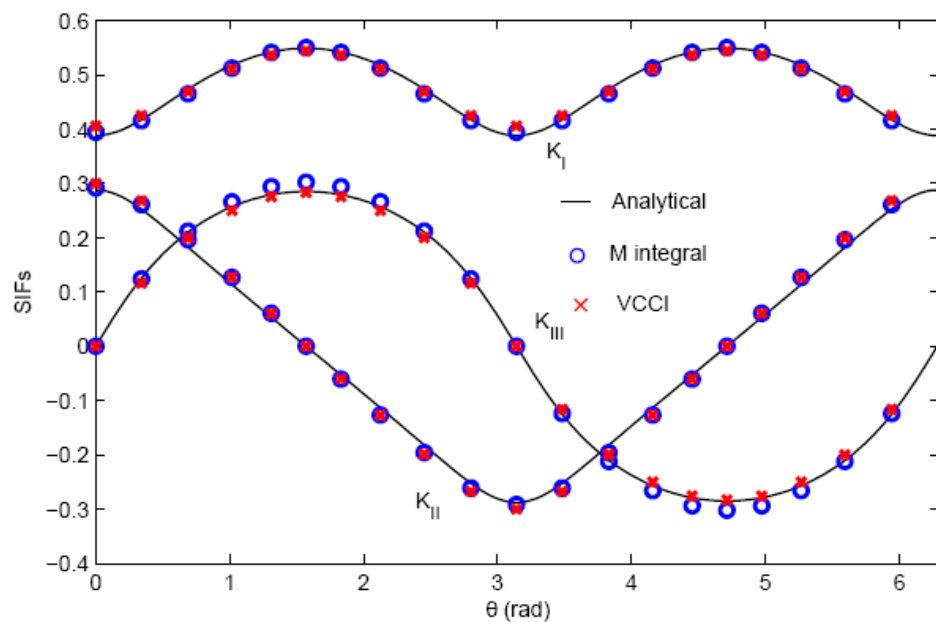
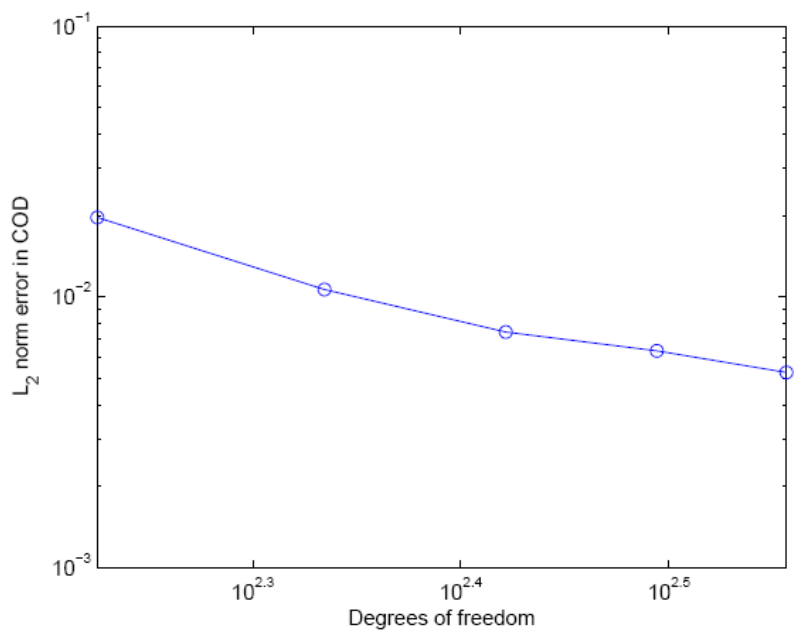


(d) improved SST, $ngp_s=18$, $e_{L_2}=1.755679e-002$

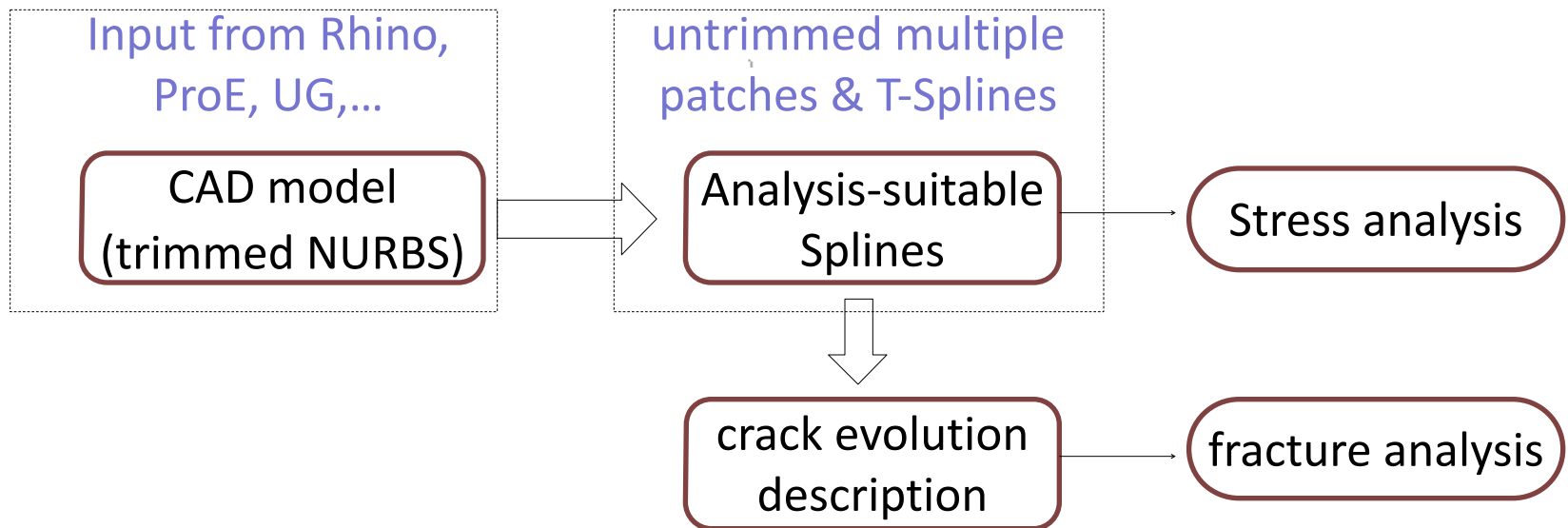
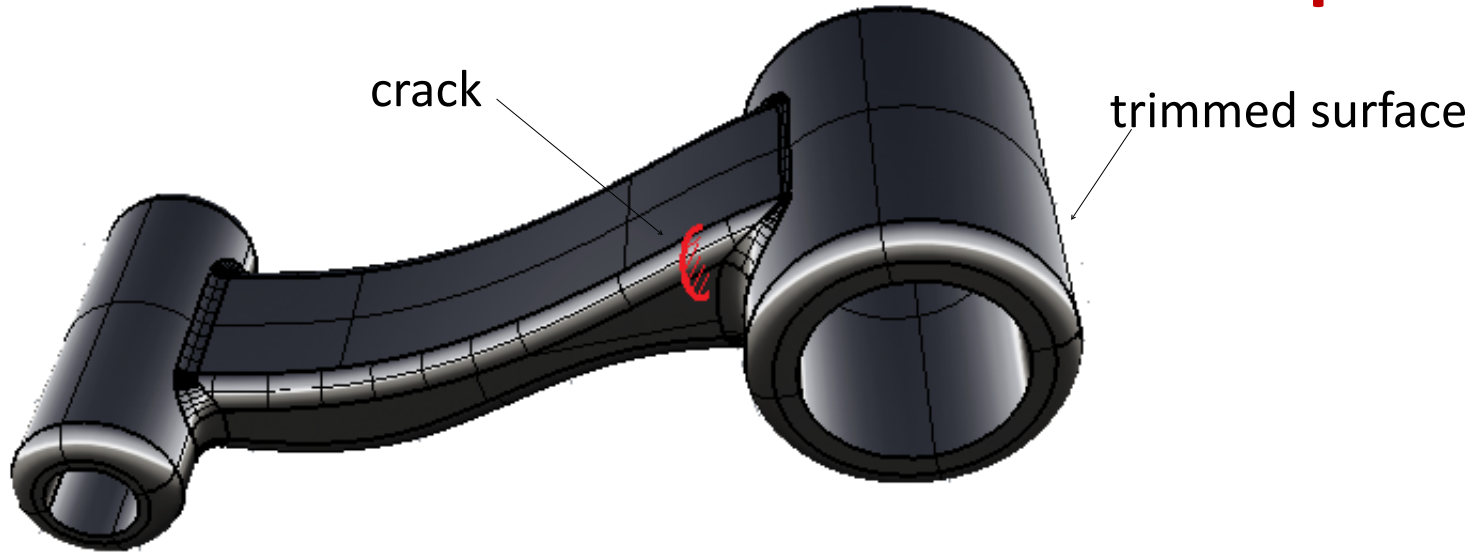


(a) original SST, $ngp_s=18$, $e_{L_2}=4.603473e-1$

(b) improved SST, $ngp_s=18$, $e_{L_2}=3.798002e-2$



➤ How far are we from non-trivial 3D workpieces?



- Dual boundary integral equations combined with isogeometric analysis are used to model fracture (2D & 3D) and crack growth (2D)
- Partition of unity enrichment (2D) and graded mesh refinement (2D & 3D) are used to improve accuracy near the crack tip or crack front
- Stable quadrature scheme is proposed for singular integration in 3D. This makes the method non-sensitive to mesh distortion
- Different ways to extract stress intensity factors based on the framework of IGABEM

➔ Questions

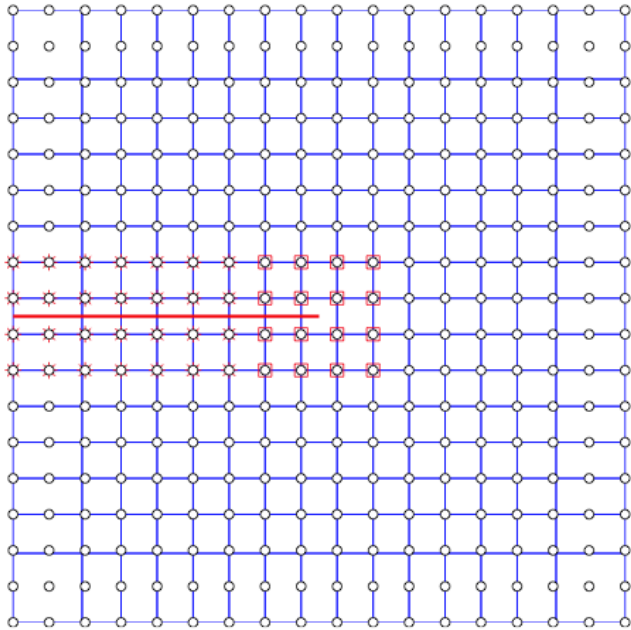
- Geometry-independent field approximation (GIFT)
- Independent displacement and traction approximations
- Independent geometry and field approximations
- Contact (BETI)
- BEM Acceleration

Handling discontinuities in isogeometric formulations

with Nguyen Vinh Phu, Marie Curie Fellow

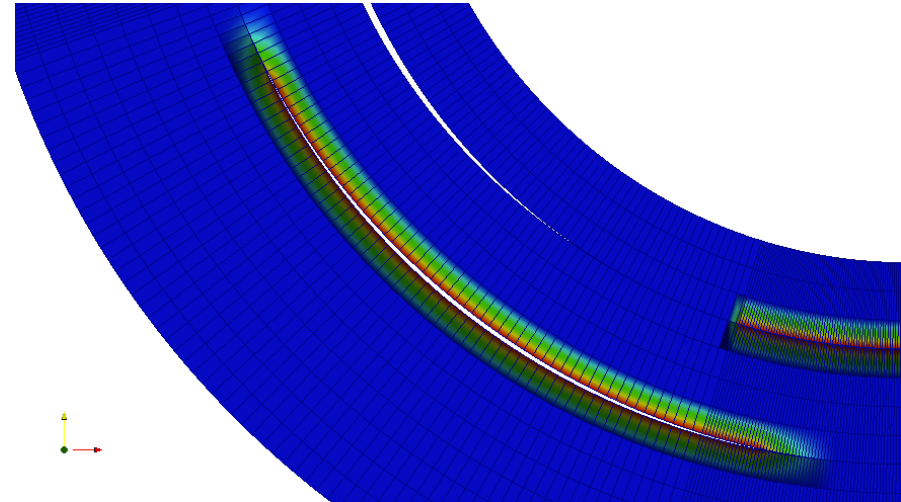


PUM enriched methods



- IGA: link to CAD and accurate stress fields
- XFEM: no remeshing

Mesh conforming methods



- IGA: link to CAD and accurate stress fields
- Apps: delamination



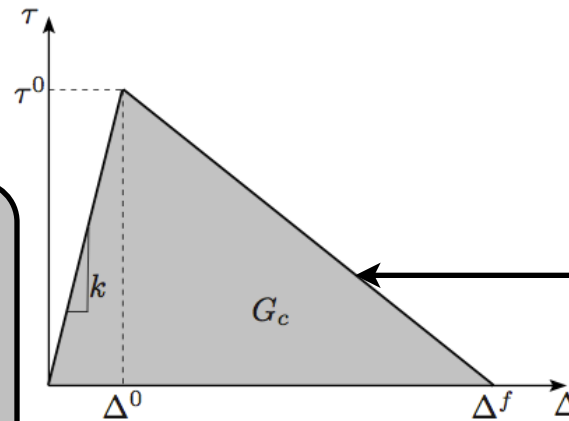
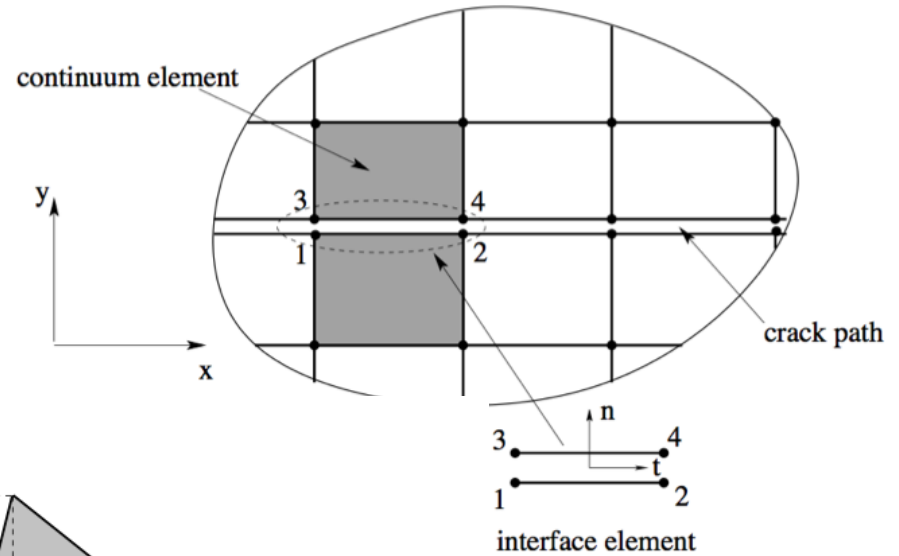
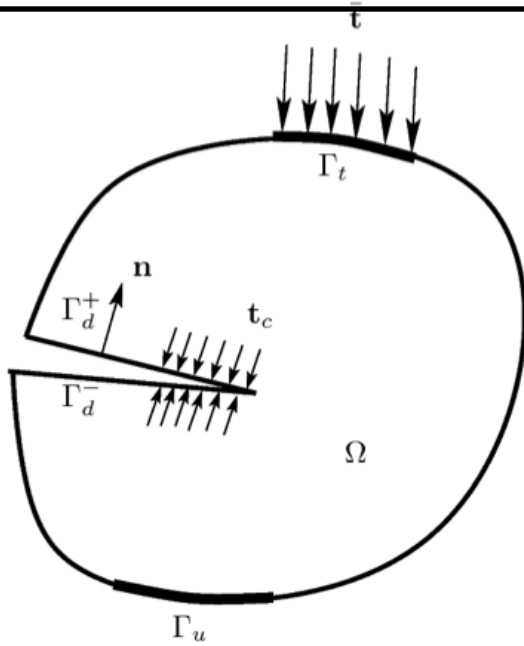
$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} R_I(\mathbf{x}) \mathbf{u}_I + \sum_{J \in \mathcal{S}^c} R_J(\mathbf{x}) \Phi(\mathbf{x}) \mathbf{a}_J$$

NURBS basis functions

enrichment functions

1. E. De Luycker, D. J. Benson, T. Belytschko, Y. Bazilevs, and M. C. Hsu. X-FEM in isogeometric analysis for linear fracture mechanics. *IJNME*, 87(6):541–565, 2011.
2. S. S. Ghorashi, N. Valizadeh, and S. Mohammadi. Extended isogeometric analysis for simulation of stationary and propagating cracks. *IJNME*, 89(9): 1069–1101, 2012.
3. D. J. Benson, Y. Bazilevs, E. De Luycker, M.-C. Hsu, M. Scott, T. J. R. Hughes, and T. Belytschko. A generalized finite element formulation for arbitrary basis functions: From isogeometric analysis to XFEM. *IJNME*, 83(6):765–785, 2010.
4. A. Tambat and G. Subbarayan. Isogeometric enriched field approximations. *CMAME*, 245–246:1 – 21, 2012.

Delamination analysis with cohesive elements (standard approach)

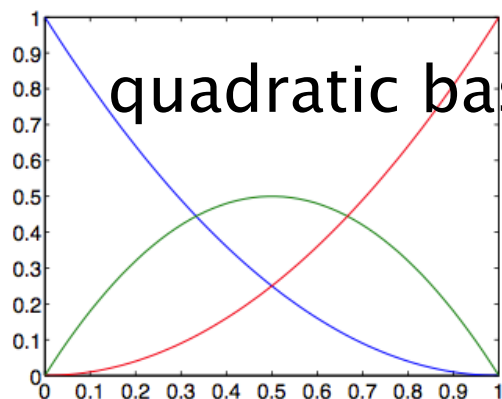


- No link to CAD
- Long preprocessing
- Refined meshes

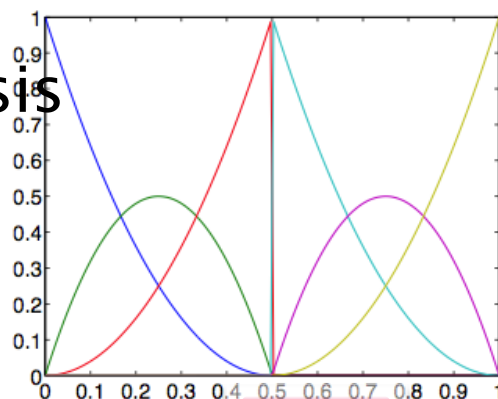
$$\int_{\Omega} \delta \mathbf{u} \cdot \mathbf{b} d\Omega + \int_{\Gamma_t} \delta \mathbf{u} \cdot \bar{\mathbf{t}} d\Gamma_t = \int_{\Omega} \delta \boldsymbol{\epsilon} : \boldsymbol{\sigma}(\mathbf{u}) d\Omega + \int_{\Gamma_d} \delta [[\mathbf{u}]] \cdot \mathbf{t}^c([[\mathbf{u}]]) d\Gamma_d$$

Isogeometric cohesive elements

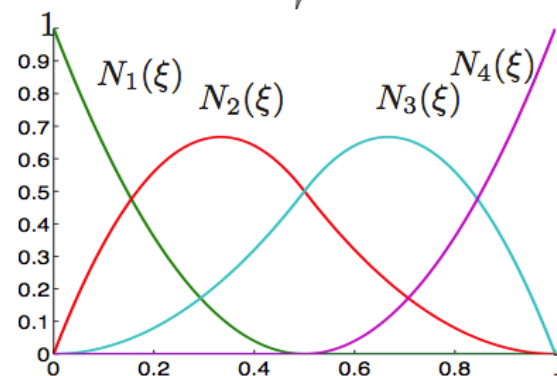
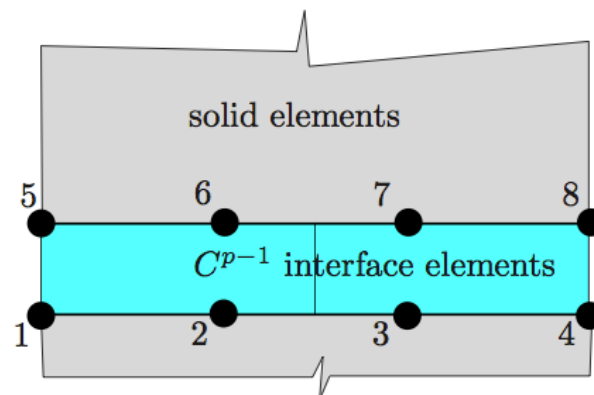
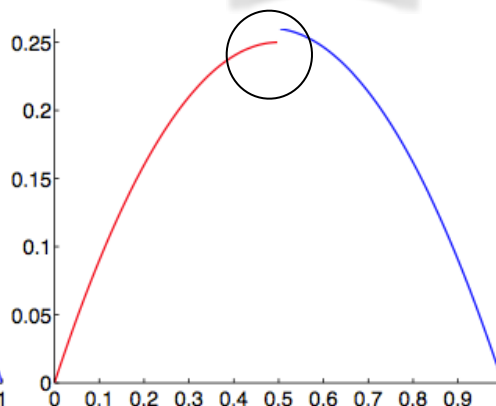
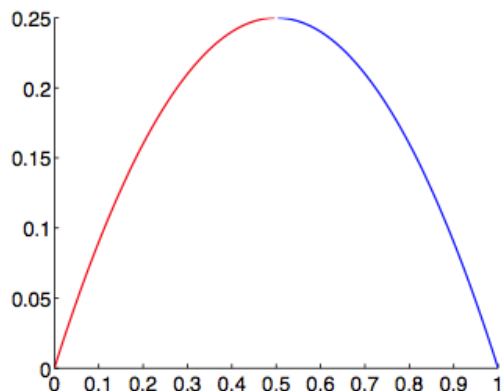
quadratic basis



(a) $\Xi = \{0, 0, 0, 1, 1, 1\}$



(b) $\Xi' = \{0, 0, 0, 0.5, 0.5, 0.5, 1, 1, 1\}$



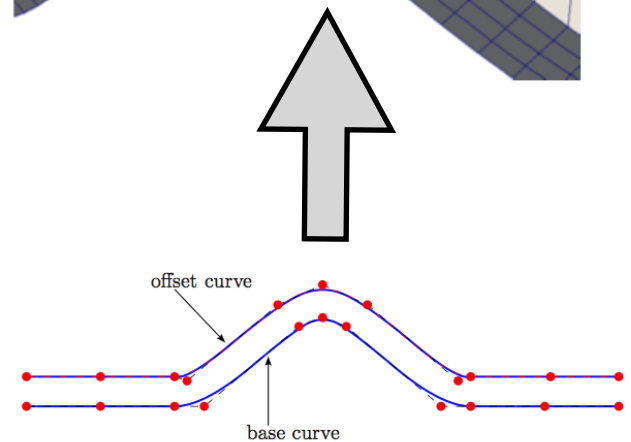
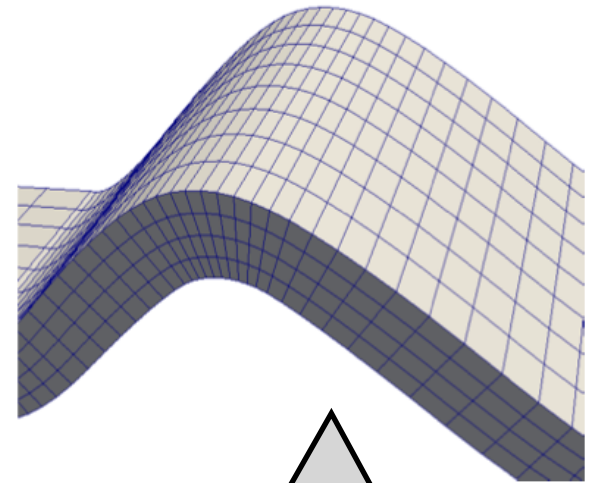
Knot insertion

1. C. V. Verhoosel, M. A. Scott, R. de Borst, and T. J. R. Hughes. An isogeometric approach to cohesive zone modeling. *IJNME*, 87(15):336–360, 2011.
2. V.P. Nguyen, P. Kerfriden, S. Bordas. Isogeometric cohesive elements for two and three dimensional composite delamination analysis, 2013, Arxiv.

Isogeometric cohesive elements: advantages

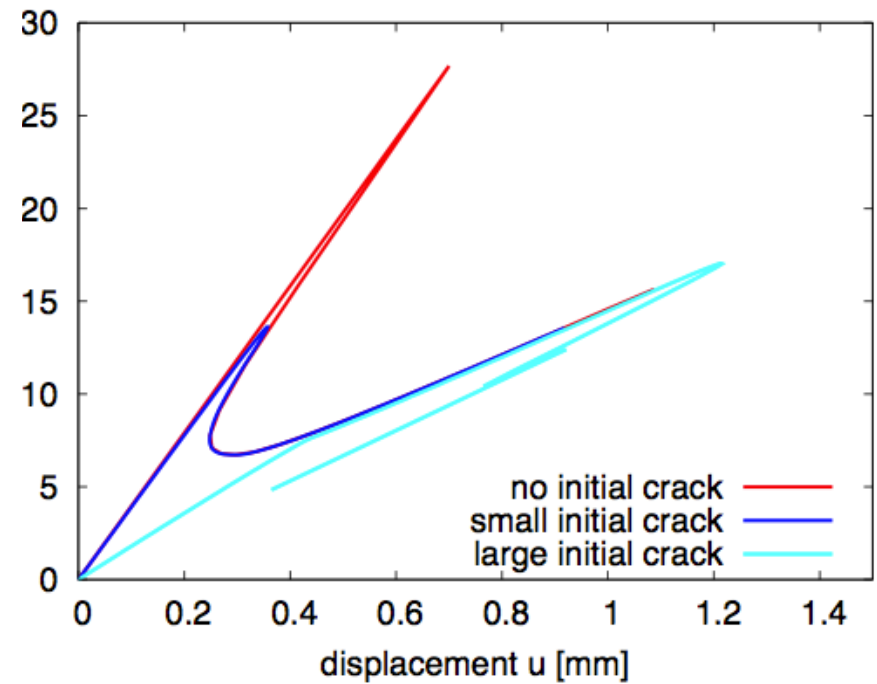
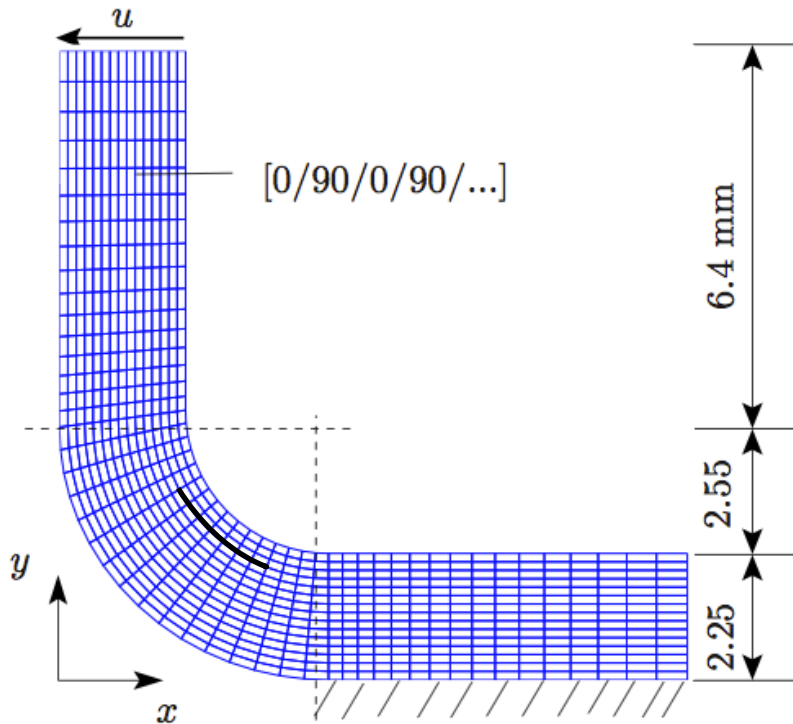
- Direct link to CAD
- Exact geometry
- Fast/straightforward generation of interface elements
- Accurate stress field
- Computationally cheaper

- 2D Mixed mode bending test (MMB)
- 2 x 70 quartic-linear B-spline elements
- Run time on a laptop 4GBi7: 6 s
- Energy arc-length control

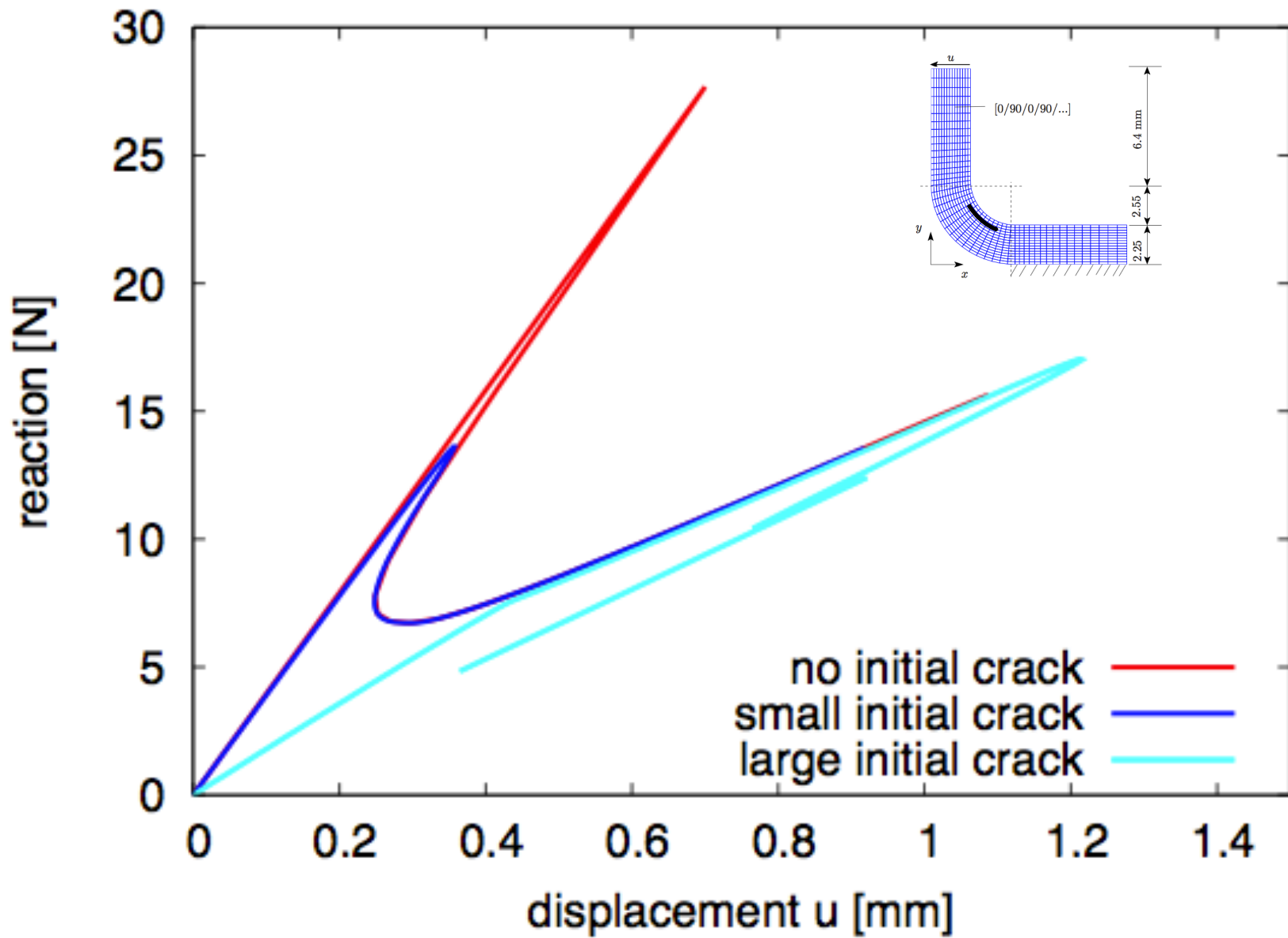


V. P. Nguyen and H. Nguyen-Xuan. High-order B-splines based finite elements for delamination analysis of laminated composites. *Composite Structures*, 102:261–275, 2013.

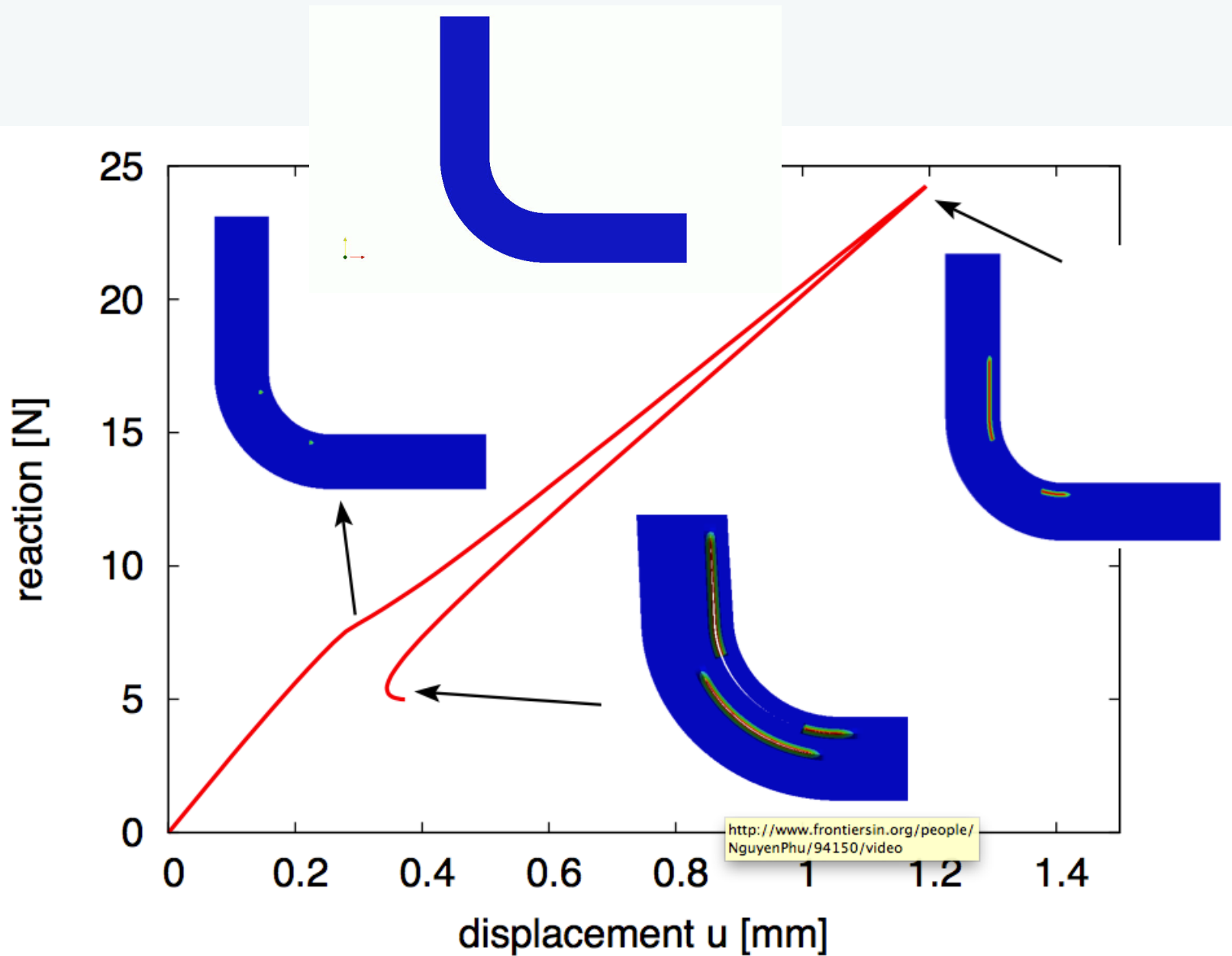
Isogeometric cohesive elements: 2D example



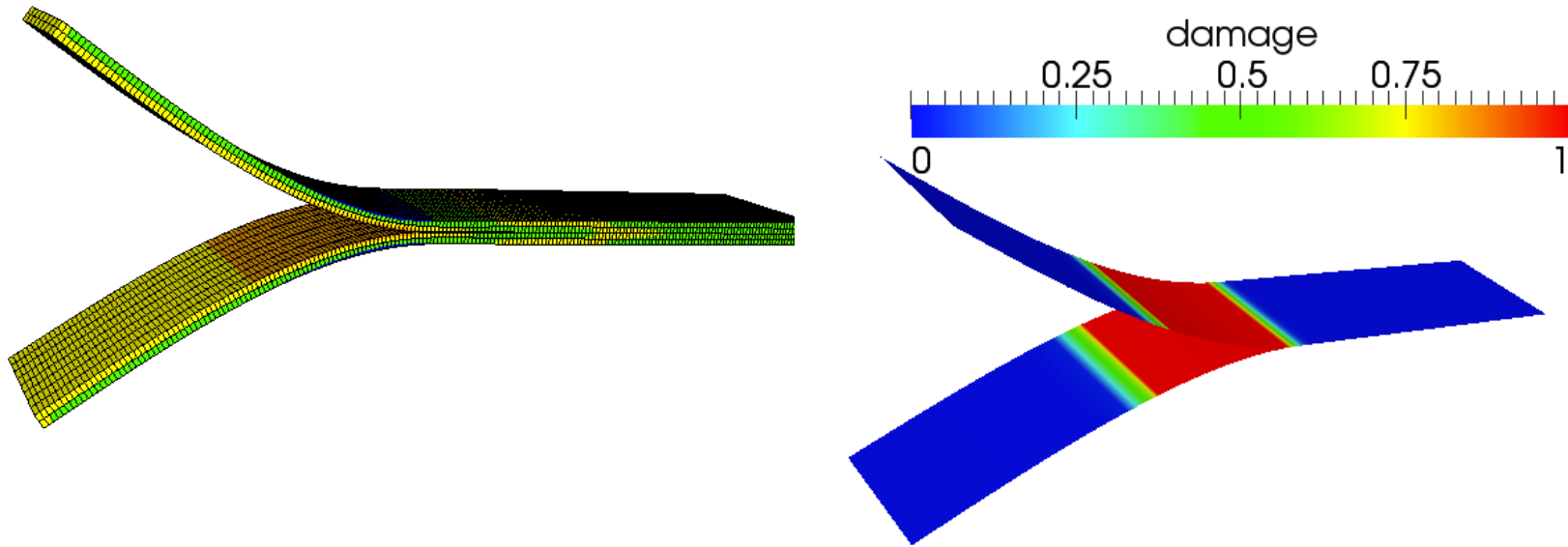
- Exact geometry by NURBS + direct link to CAD
- It is straightforward to vary
 - (1) the number of plies and
 - (2) # of interface elements:
- Suitable for parameter studies/design
- Solver: energy-based arc-length method (Gutierrez, 2007)



Isogeometric cohesive elements: 2D example

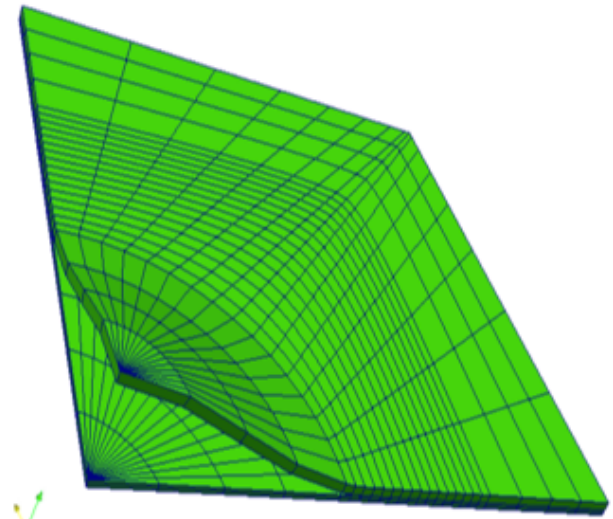
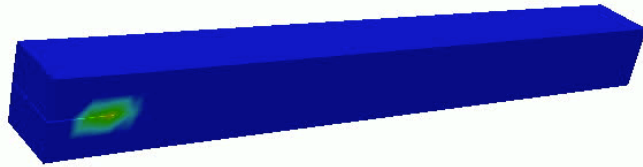


Isogeometric cohesive elements: 3D example with shells

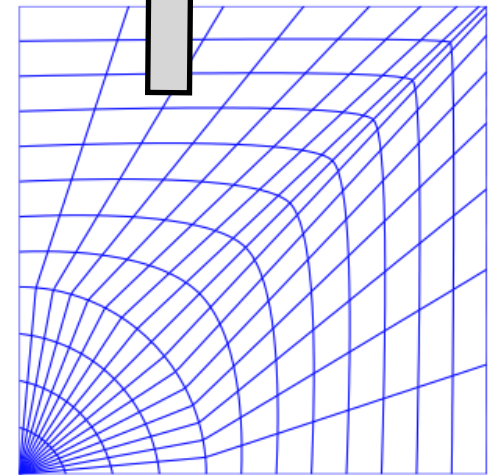
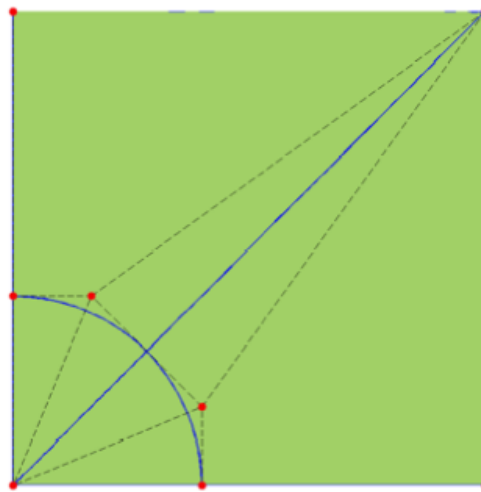


- Rotation free B-splines shell elements (Kiendl et al. CMAME)
- Two shells, one for each lamina
- Bivariate B-splines cohesive interface elements in between

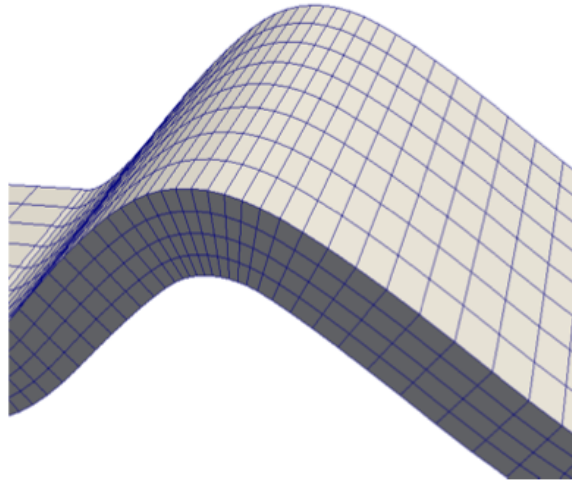
Isogeometric cohesive elements: 3D examples



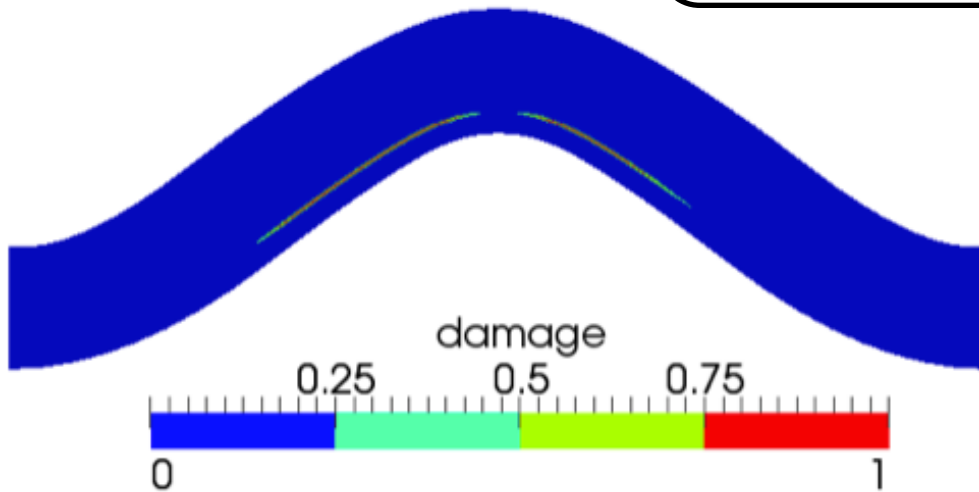
- cohesive elements for 3D meshes the same as 2D
- large deformations



Isogeometric cohesive elements



- singly curved thick-wall laminates
- geometry/displacements: NURBS
- trivariate NURBS from NURBS surface(*)
- cohesive surface interface elements



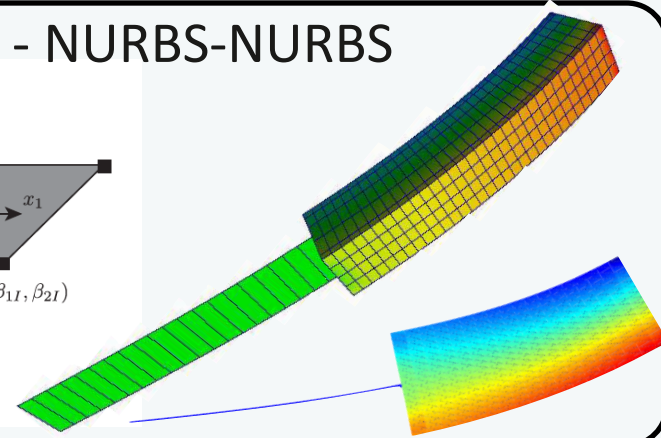
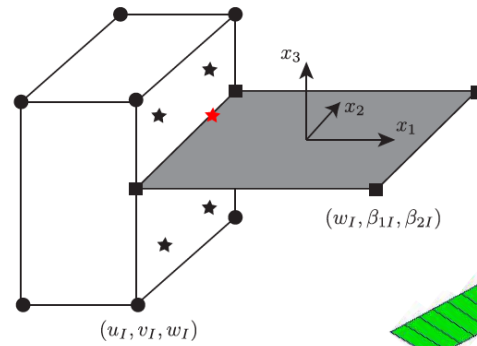
(*)V. P. Nguyen, P. Kerfriden, S.P.A. Bordas, and T. Rabczuk. An integrated design-analysis framework for three dimensional composite panels. Computer Aided Design, 2013. submitted.

Future work: model selection (continuum, plate, beam, shell?)

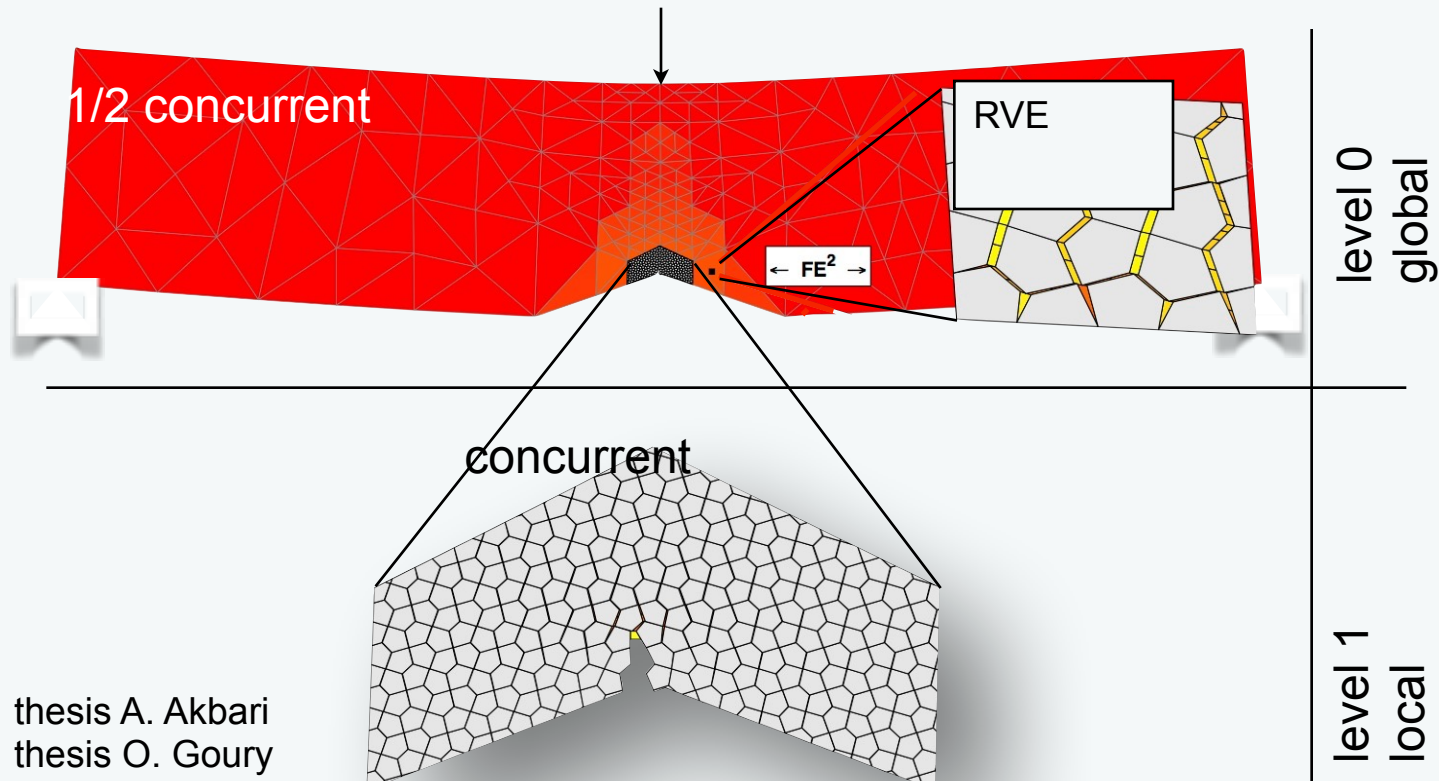
Model selection

- Model with shells
- Identify “hot spots” - dual
- Couple with continuum
- Coarse-grain

• Nitsche coupling - NURBS-NURBS



load



Thank you for your attention!

International Centre
for Mechanical Sciences



CISM-ECCOMAS International Summer School on “Modelling, Simulation and Characterization of Multi-Scale Heterogeneous Materials” September 28, 2015 — October 2, 2015

OPEN SOURCE CODES

PERMIX: Multiscale, XFEM, large deformation, coupled 2 LAMMPS, ABAQUS, OpenMP -

MATLAB Codes: XFEM, 3D ISOGOMETRIC XFEM, 2D ISOGOMETRIC BEM, 2D MESHLESS
DOWNLOAD @ <http://cmechanicsos.users.sourceforge.net/>

COMPUTATIONAL MECHANICS DISCUSSION GROUP Request membership @
http://groups.google.com/group/computational_mechanics_discussion/about

Part III. Application to multi-crack propagation

with Danas Sutula, President Scholar



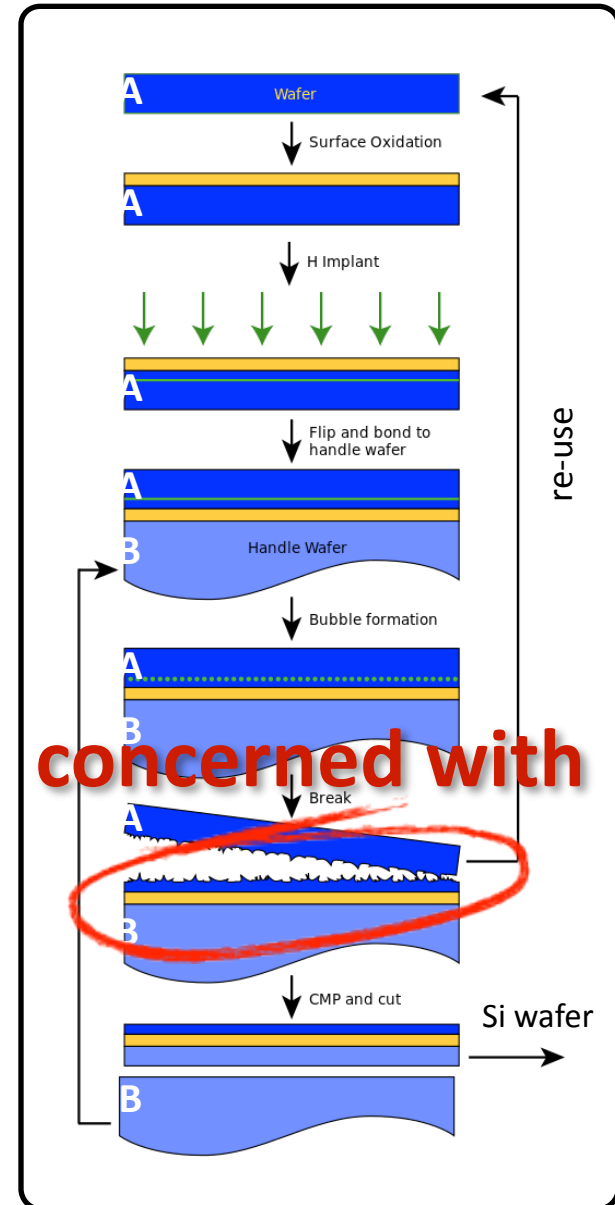
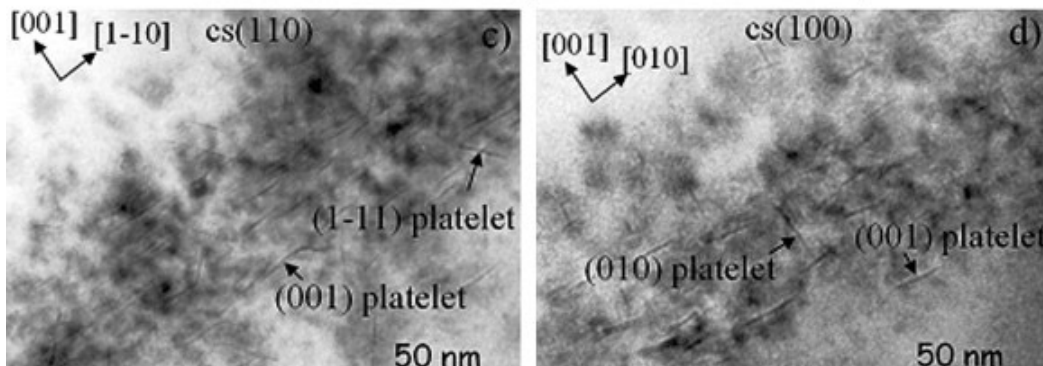
Soitec

Numerical Modeling of SOI Wafer Splitting



Manufacturing process: *SmartCut*TM

- H⁺ ionization of a thin surface of Si
- Bonding to a handle-wafer (stiffener)
- High temperature thermal annealing
- Nucleation and growth of cavities filled with H₂
- Pressure driven micro crack growth
- Coalescence and post-split fracture roughness



Determine:

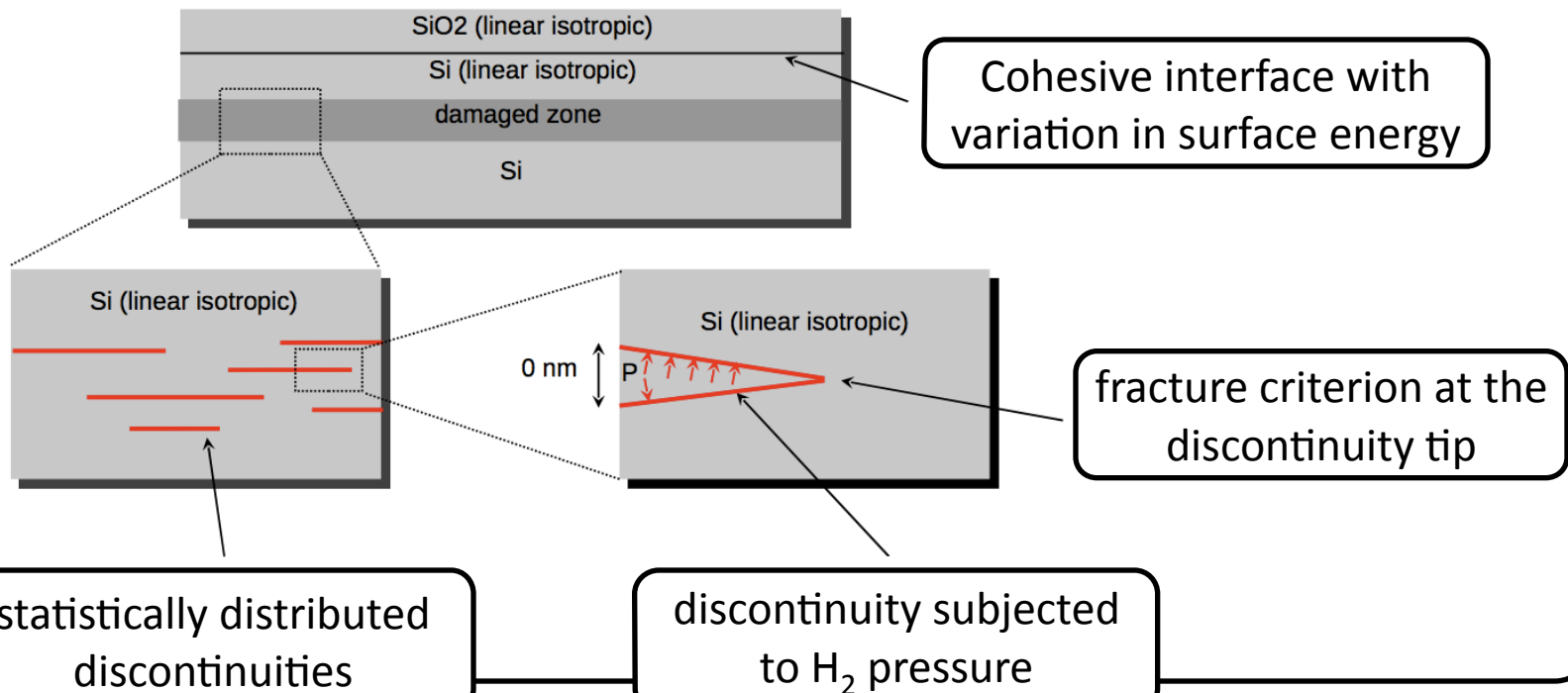
- micro crack nucleation points and direction
- multiple crack paths until coalescence
- time to complete fracture
- final surface roughness

Modeling cavities by zero thickness surfaces

- discontinuities in the displacement field

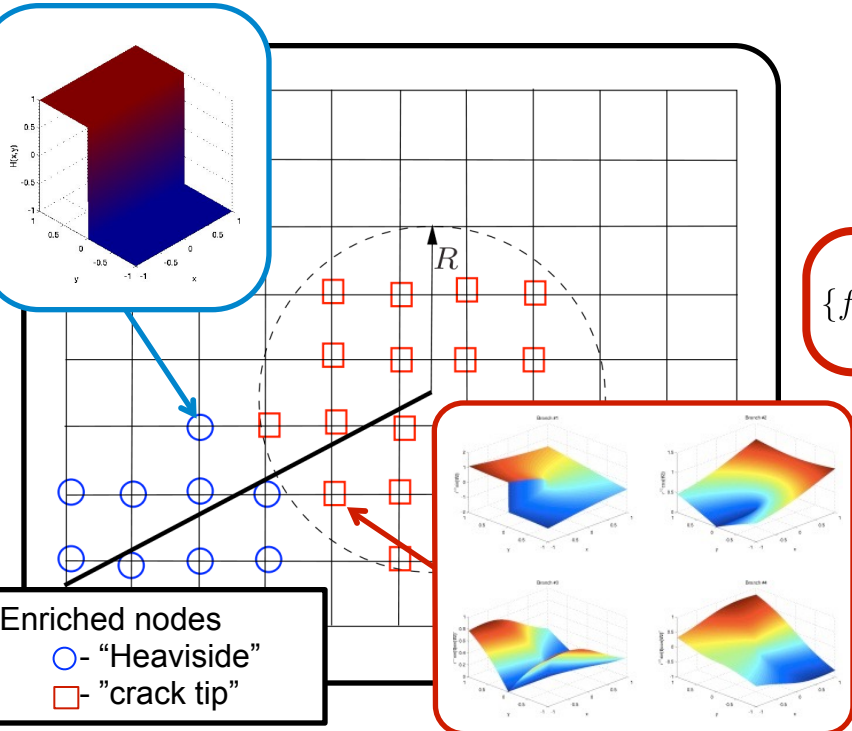
Linear elastic fracture mechanics (LEFM)

- infinite stress at crack tip, i.e. *singularity*



Approximation function:

$$\mathbf{u}^h(\mathbf{x}) = \underbrace{\sum_{I \in \mathcal{N}_I} N_I(\mathbf{x}) \mathbf{u}^I}_{\text{standard part}} + \underbrace{\sum_{J \in \mathcal{N}_J} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}^J}_{\text{discontinuous enrichment}} + \underbrace{\sum_{K \in \mathcal{N}_K} N_K(\mathbf{x}) \sum_{\alpha=1}^4 f_\alpha(\mathbf{x}) \mathbf{b}^{K\alpha}}_{\text{singular tip enrichment}}$$



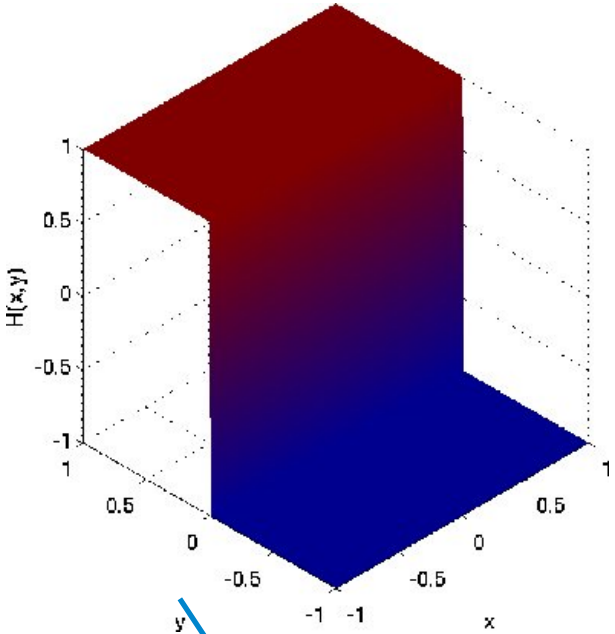
$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{x} \text{ above crack} \\ -1 & \text{if } \mathbf{x} \text{ below crack} \end{cases}$$

$$\{f_\alpha(r, \theta), \alpha = 1, 4\} = \left\{ \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2} \sin \theta, \sqrt{r} \cos \frac{\theta}{2} \sin \theta \right\}$$

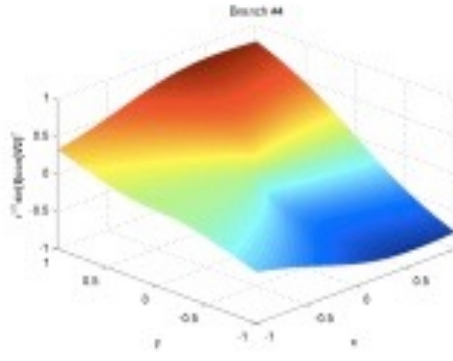
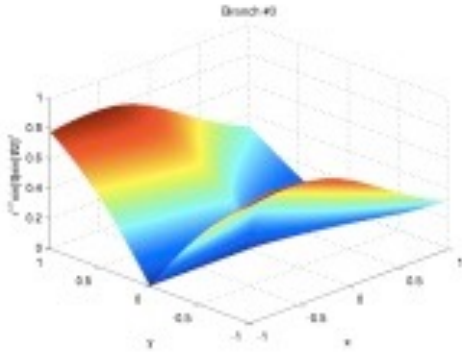
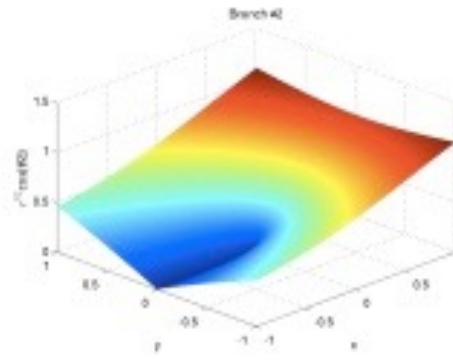
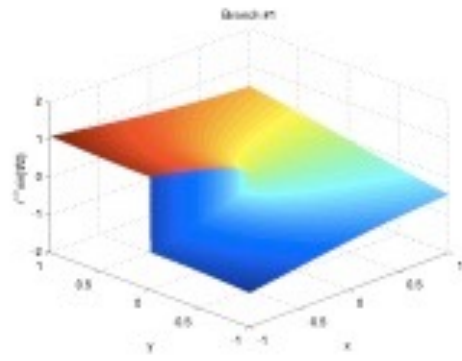
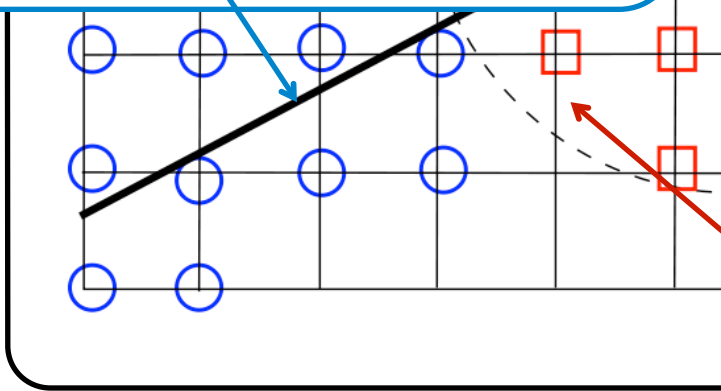
Enriched nodes
 ○ - "Heaviside"
 □ - "crack tip"

XFEM formulation

$$H(x) = \begin{cases} +1 & \text{if } x \text{ above crack} \\ -1 & \text{if } x \text{ below crack} \end{cases}$$



$$B(r, \theta) = \left\{ \sqrt{r} \cos \frac{\theta}{2} \quad \sqrt{r} \sin \frac{\theta}{2} \quad \sqrt{r} \sin \theta \sin \frac{\theta}{2} \quad \sqrt{r} \sin \theta \cos \frac{\theta}{2} \right\}$$



Extended Finite Element Method (XFEM)

- Introduced by Ted Belytschko (1999) for elastic problems

Fracture of “XFEM” using XFEM

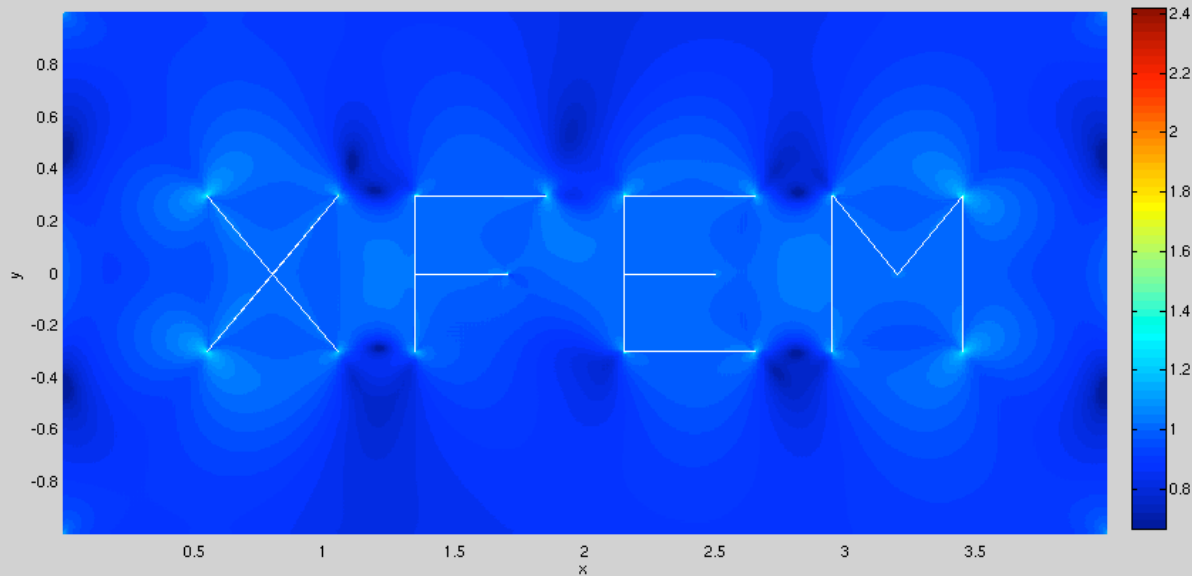
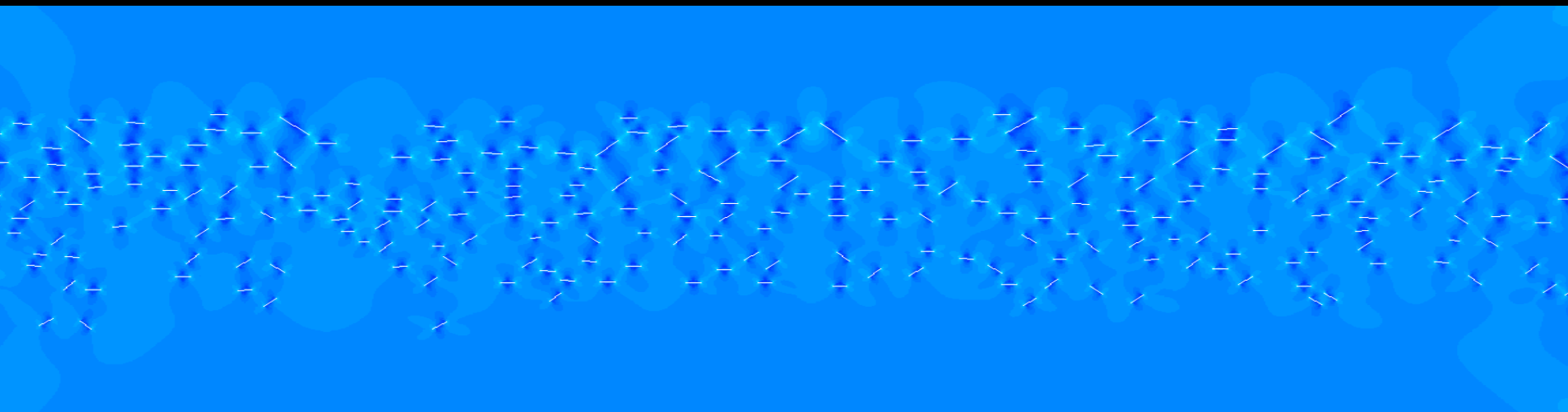
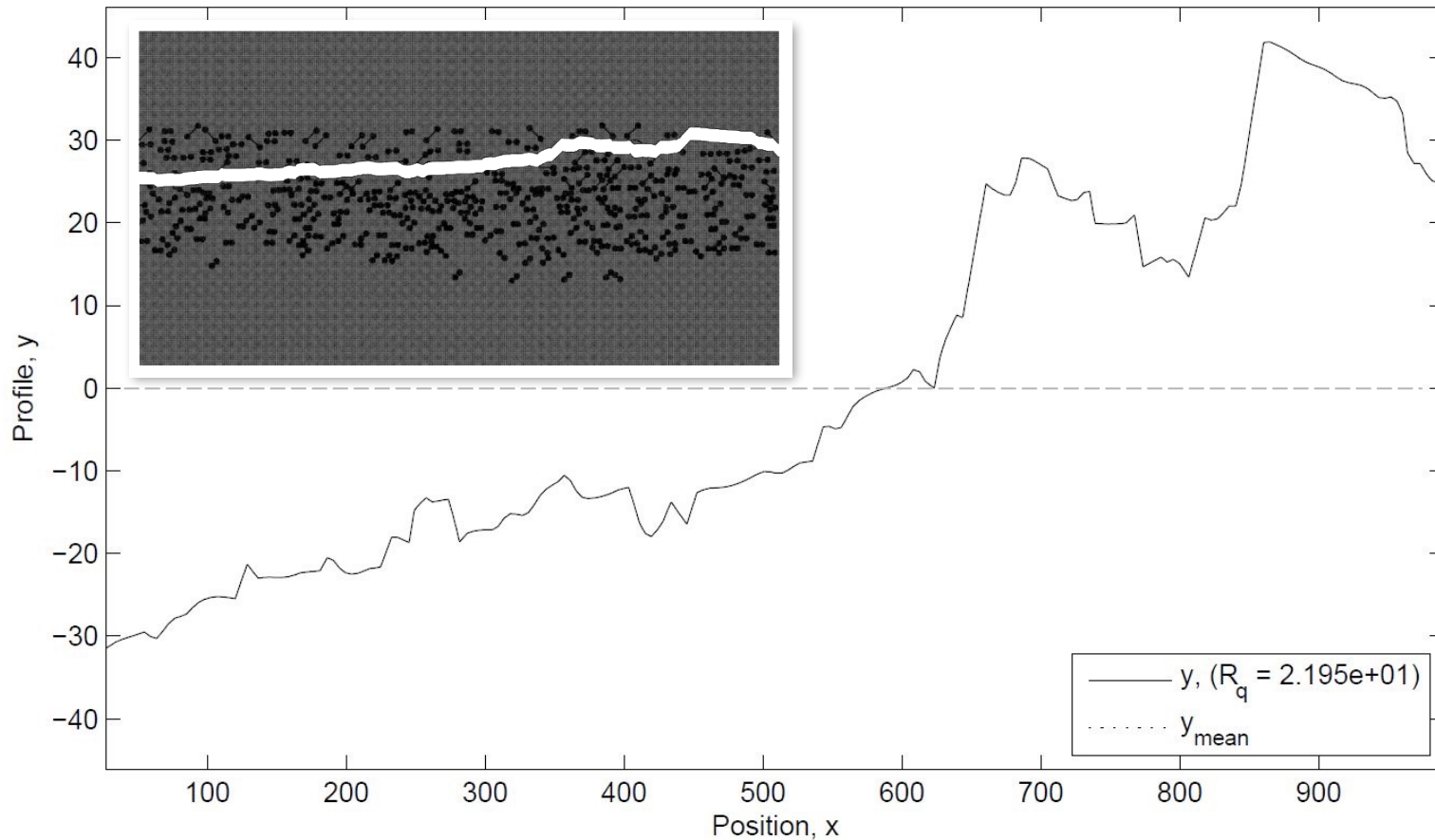


Plate with 300 cracks - vertical extension BCs



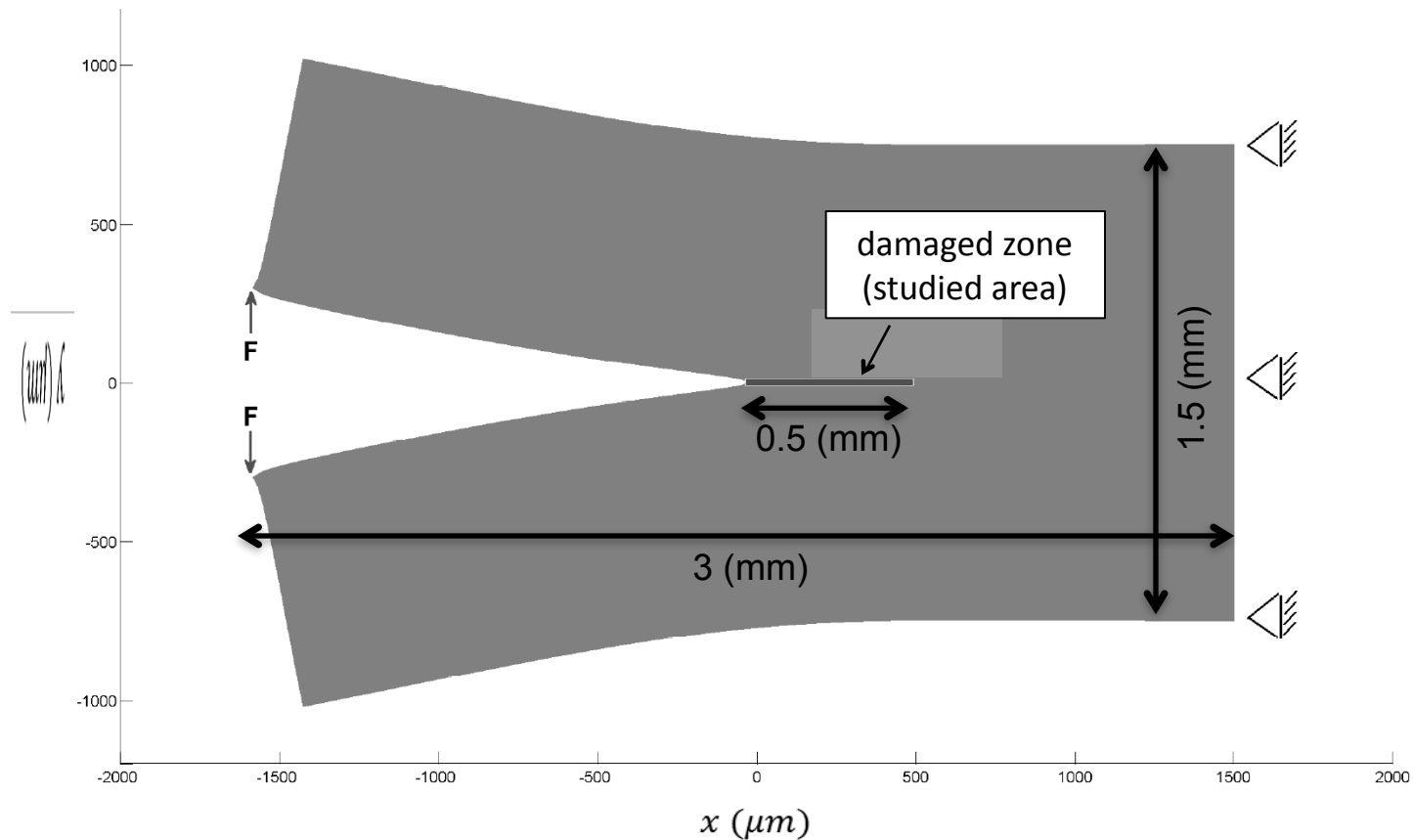
Vertical extension of a plate with 300 cracks

Post-split roughness



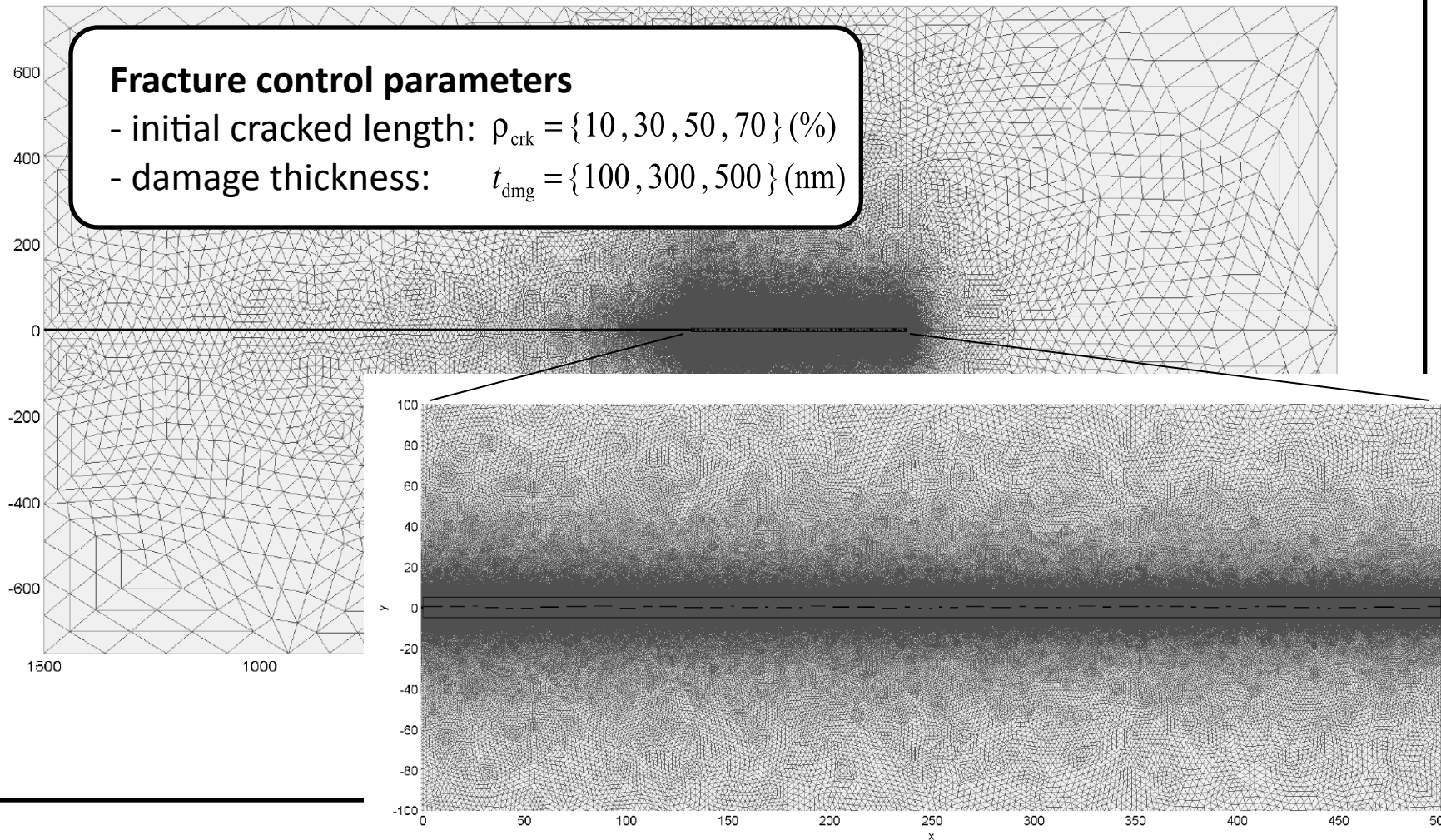
Mechanical splitting of a wafer sample

- Post-split roughness as a function of micro crack distribution



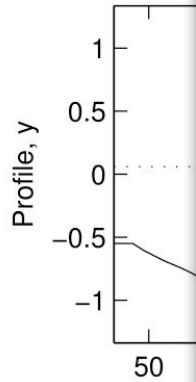
Mechanical splitting of a wafer sample

- Discretisation (≈ 1 mln. DOF, $h_e = 150$ nm)

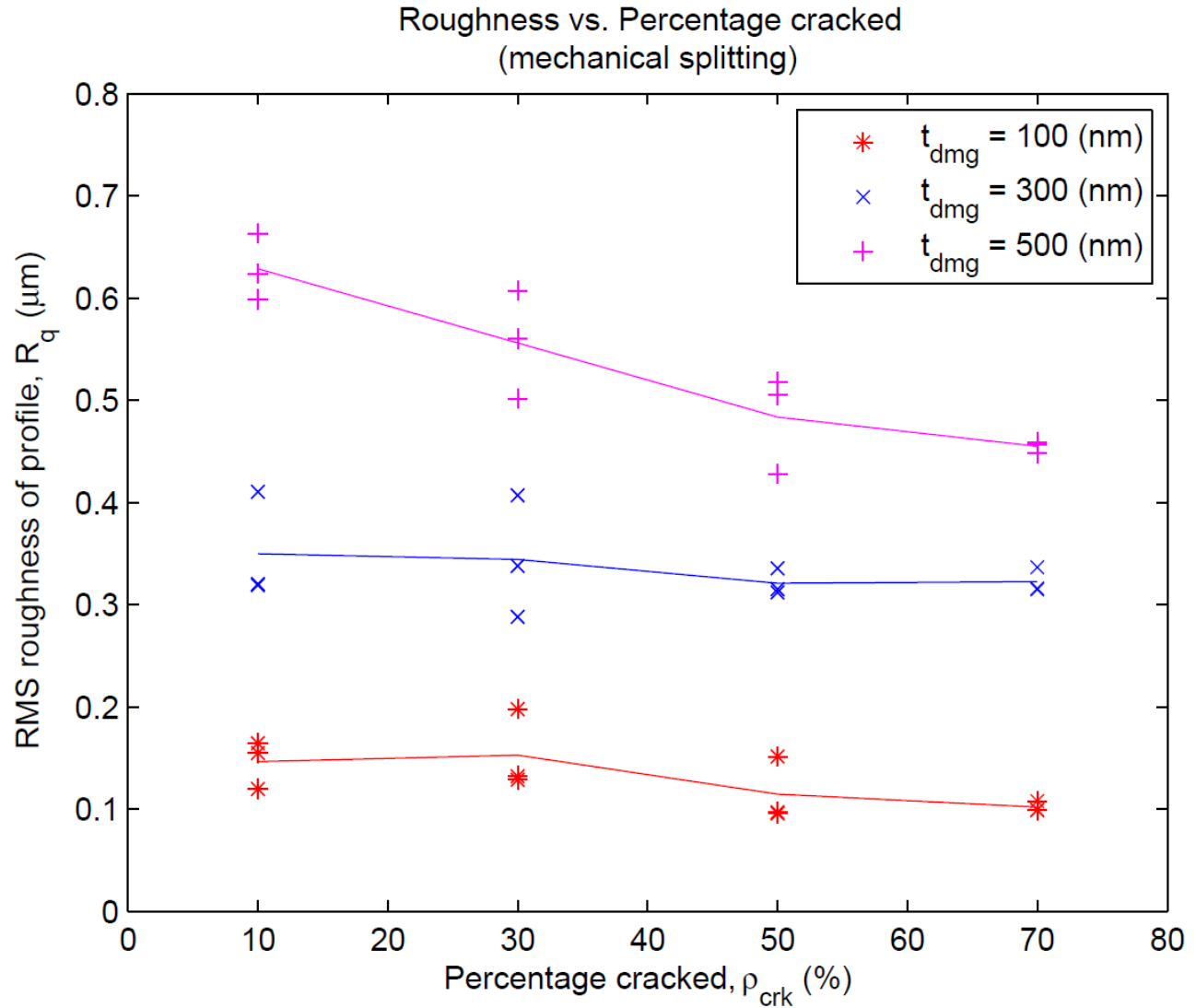
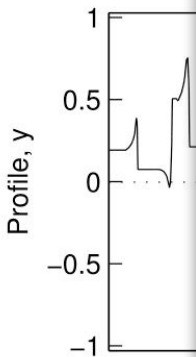


Fracture ro

- Case exa



- Case exa



Part IV. Application to surgical simulation

with INRIA, France; Karol Miller, UWA.



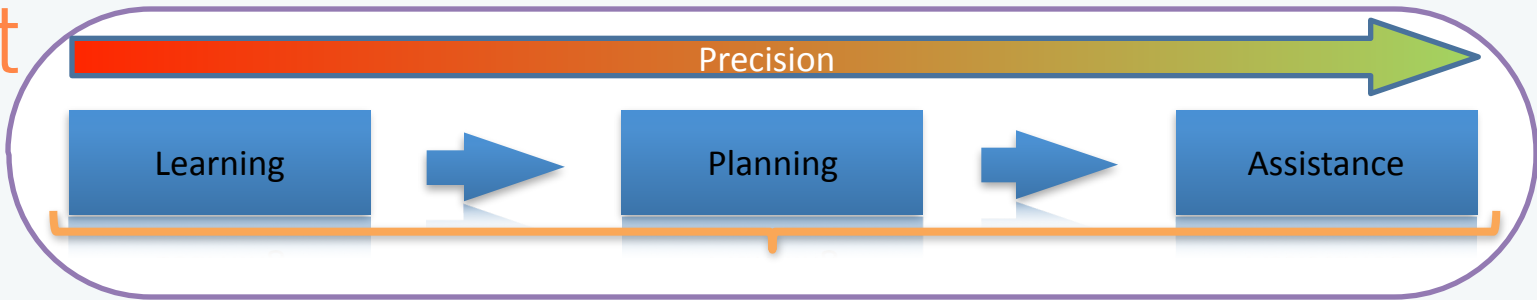
RealTcut

149

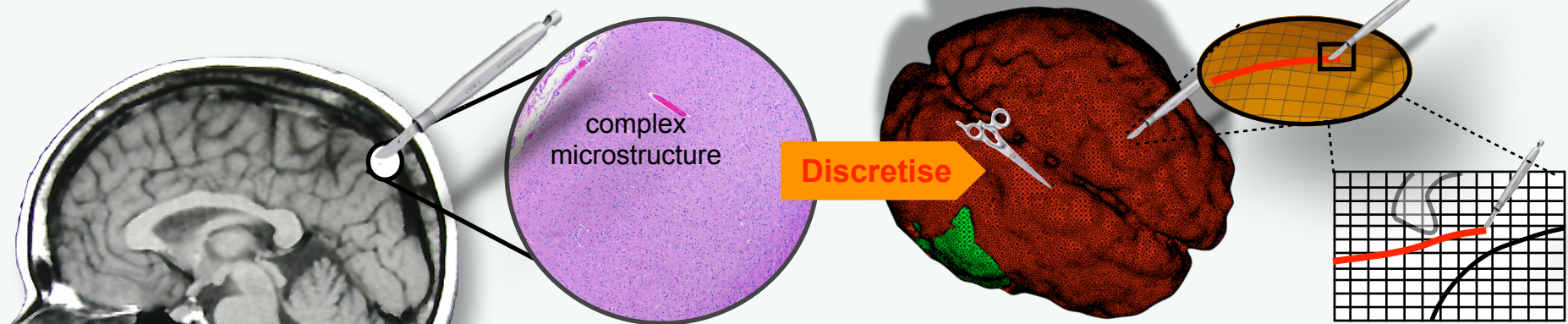
**Interactive multiscale
cutting simulations**



RealTcut

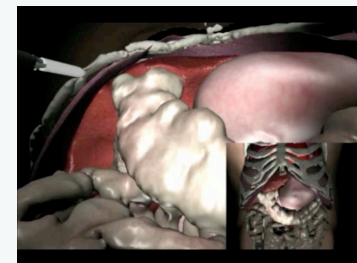
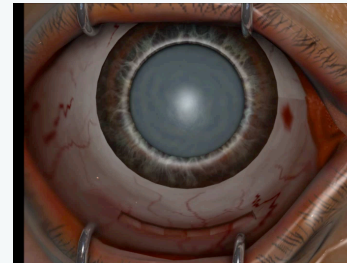
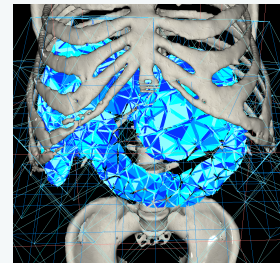
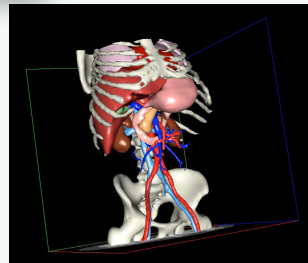


Surgical simulation (real time/interactivity)



- ▶ Reduce the problem size while controlling error in solving very large multiscale mechanics problems

Courteuisse et al. PBMB 2011

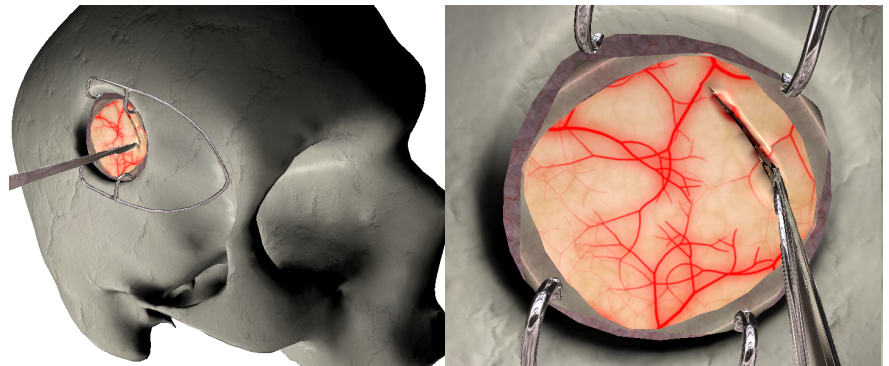


Concrete objective: compute the response of organs during surgical procedures (including cuts) in real time (50-500 solutions per second)

Two schools of thought

- ▶ constant time
 - ➔ accuracy often controlled visually only
- ▶ model reduction or “learning”
 - ➔ scarce development for biomedical problems
 - ➔ no results available for cutting

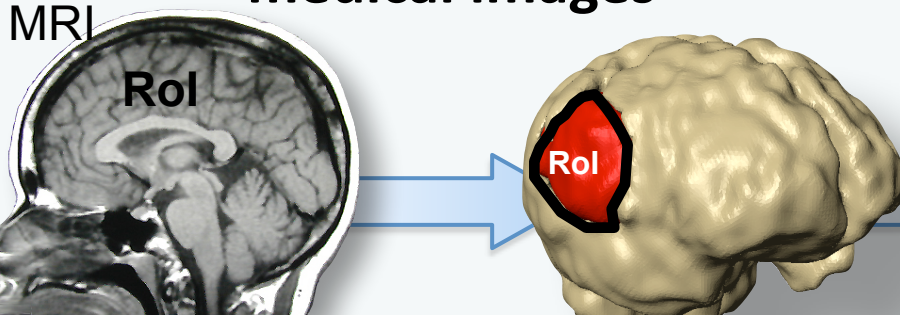
First implicit, interactive method for cutting with contact



[Courtecuisse et al., MICCAI, 2013]
Collaboration INRIA

Proposed approach: maximize accuracy for given computational time. Error control

Complex geometries from medical images



segmentation

Region of interest (RoI)

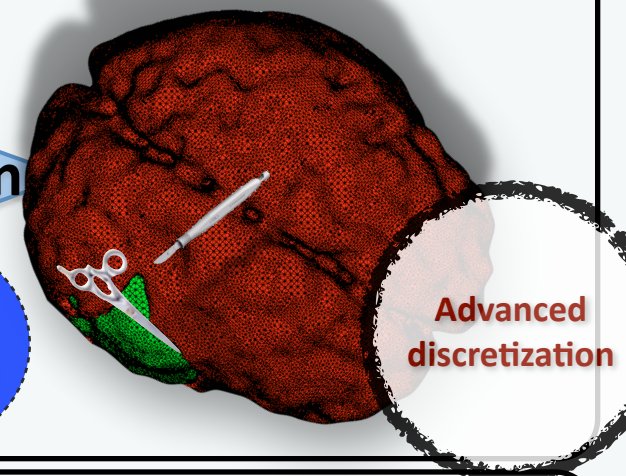
Topological changes & contact

discretization

Model reduction

Advanced discretization

adaptive



Error control

- interactivity
- space-time discretization?
- optimize use of compute resources

Verification & Validation



A semi-implicit method for real-time deformation, topological changes, and contact of soft tissues

Paper ID : 269

**TWO POST DOCS
TWO FACULTY POSITIONS AVAILABLE**

OPEN SOURCE CODES

PERMIX: Multiscale, XFEM, large deformation, coupled 2 LAMMPS, ABAQUS, OpenMP -
Fortran 2003, C++

MATLAB Codes: XFEM, 3D ISOGEOMETRIC XFEM, 2D ISOGEOMETRIC BEM, 2D MESHLESS
DOWNLOAD @ <http://cmechanicsos.users.sourceforge.net/>

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