Problem statement: parametrized weak form

- Exact parametrized elastodynamic problem

$$m\left(\frac{\partial^2 u^e(x,t;\underline{\mu})}{\partial t^2}, v; \underline{\mu}\right) + c\left(\frac{\partial u^e(x,t;\underline{\mu})}{\partial t}, v; \underline{\mu}\right) + a\Big(u^e(x,t;\underline{\mu}), v; \underline{\mu}\Big) = g(t) f(v;\underline{\mu}),$$

$$\forall v \in \left(H_0^1(\Omega)\right)^d, t \in [0,T], \underline{\mu} \in \mathcal{D}$$

- Initial conditions: $u_i^e(x,0;\underline{\mu}) = 0; \ \dfrac{\partial u_i^e}{\partial t}(x,0;\underline{\mu}) = 0$
- Boundary conditions: $u_i^e\left(x,t;\underline{\mu}\right) = 0, \ \forall x \in \partial\Omega_D$

$$\sigma_{ij}^e\left(x,t;\underline{\mu}\right)\hat{n}_j = \mathsf{t}_i, \ \forall x \in \partial\Omega_N$$

- Space-time quantity of interest:

$$s^e(\underline{\mu}) = \int_0^T \int_{\Gamma_o} u^e(x,t;\underline{\mu}) \Sigma(x,t) \, dx dt = \int_0^T \ell\Big(u^e(x,t;\underline{\mu})\Big) \, dt$$

$$\underline{\mu}\Big(\rightarrow u^e(\underline{\mu})\Big) \rightarrow s^e(\underline{\mu})?$$

Problem statement…

- Bi/linear forms

$$m\left(w,v;\underline{\mu}\right)=\sum_i\int_\Omega \rho v_i\,\frac{\partial^2 w_i}{\partial t^2}\,d\Omega$$

$$c\left(w,v;\underline{\mu}\right)=\sum_i\int_\Omega \alpha\rho v_i w_i d\Omega+\sum_{i,j,k,l}\int_\Omega \beta\,\frac{\partial v_i}{\partial x_j}C_{ijkl}\,\frac{\partial w_k}{\partial x_l}\,d\Omega$$

$$a\left(w,v;\underline{\mu}\right)=\sum_{i,j,k,l}\int_\Omega \frac{\partial v_i}{\partial x_j}C_{ijkl}\,\frac{\partial w_k}{\partial x_l}\,d\Omega$$

$$f\left(v;\underline{\mu}\right)=\sum_i\int_\Omega b_i v_i\,d\Omega+\sum_i\int_{\partial\Omega_{\mathrm{N}}} v_i \mathsf{t}_i\,d\Gamma$$

- Bilinear forms m, a are continuous and coercive.
- Assume affine parameter dependence of the bi/linear forms

Finite element discretization

Trapezoidal scheme

- “Method of Lines”: spatial discretize (FE) + temporal discretize (Newmark)
  - Discretize the time span $[0,T]$ into $[t^k, t^{k+1}], \quad 0 \le k \le K-1$
  - Solve $(K-1)$ following elliptic systems

$$\boxed{\underline{\underline{\mathcal{A}}}\left(\underline{u}^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu}\right) = \underline{\mathcal{F}}(\underline{v}),} \qquad \forall \underline{v} \in Y^{\mathrm{h}}, \underline{\mu} \in \mathcal{D}, \;\; 1 \le k \le K-1$$

$$\left\{\begin{aligned}
\underline{\underline{\mathcal{A}}}\left(\underline{u}^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu}\right) &= \frac{1}{\Delta t^2} m(\underline{u}^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu}) + \frac{1}{2\Delta t} c(\underline{u}^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu}) + \frac{1}{4} a(\underline{u}^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu}) \\
\underline{\mathcal{F}}(\underline{v}) &= -\frac{1}{\Delta t^2} m(\underline{u}^{k-1}(\underline{\mu}), \underline{v}; \underline{\mu}) + \frac{1}{2\Delta t} c(\underline{u}^{k-1}(\underline{\mu}), \underline{v}; \underline{\mu}) - \frac{1}{4} a(\underline{u}^{k-1}(\underline{\mu}), \underline{v}; \underline{\mu}) \\
&\quad + \frac{2}{\Delta t^2} m(\underline{u}^{k}(\underline{\mu}), \underline{v}; \underline{\mu}) - \frac{1}{2} a(\underline{u}^{k}(\underline{\mu}), \underline{v}; \underline{\mu}) + g^{eq}(t^k) f(\underline{v}; \underline{\mu}) \\
u(\underline{\mu}, t^0) &= 0; \quad \frac{\partial \underline{u}(\underline{\mu}, t^0)}{\partial t} = 0
\end{aligned}\right.$$

$$\boxed{\underline{\mu}\left(\rightarrow \underline{u}(\underline{\mu})\right) \rightarrow s(\underline{\mu})?}$$

  - FE quantity of interest: $s(\underline{\mu}) = \sum_{k=0}^{K-1} \int_{t^k}^{t^{k+1}} \ell\left(\underline{u}(x,t;\underline{\mu})\right) dt$

RB approximation: Galerkin projection

- Introduce $S_* = \{\underline{\mu}_1 \in \mathcal{D}, \underline{\mu}_2 \in \mathcal{D}, \ldots, \underline{\mu}_N \in \mathcal{D}\},\ 1 \le N \le N_{\max}$; and nested Lagrangian RB spaces

$$Y_N = \operatorname{span}\{\underline{\zeta}_n, 1 \le n \le N\},\ 1 \le N \le N_{\max}$$

–Galerkin projection:

$$\underline{u}_N(\underline{\mu}, t^k) = \sum_{n=1}^{N} u_{N\,n}(\underline{\mu}, t^k)\,\underline{\zeta}_n, \quad \forall \underline{\zeta}_n \in Y_N,\ 1 \le k \le K$$

–Solve the following elliptic systems

$$\boxed{\underline{\underline{\mathcal{A}}}\Big(\underline{u}_N^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu}\Big) = \underline{\mathcal{F}}(\underline{v}),}\ \forall \underline{v} \in Y_N, \underline{\mu} \in \mathcal{D},\ 1 \le k \le K-1$$

–RB quantity of interest:

$$\boxed{\underline{\mu}\Big(\rightarrow \underline{u}_N(\underline{\mu})\Big) \rightarrow s_N(\underline{\mu})?}$$

$$s_N(\underline{\mu}) = \sum_{k=0}^{K-1} \int_{t^k}^{t^{k+1}} \ell\Big(\underline{u}_N(x, t; \underline{\mu})\Big)\,dt$$

Approaches to build goal-oriented basis functions?

- Dual Weighted Residual (DWR) method

  [Meyer *et al*. 2003] [Grepl *et al.* 2005]
  [Bangerth *et al*. 2001] [Bangerth *et al.* 2010]

  – Solve additionally an adjoint problem
  – Remove the snapshots cause small error – keep the ones cause large error

- Build optimal goal-oriented basis functions based on all POD snapshots [Bui *et al*. 2007] [Willcox *et al.* 2005]

  – Use adjoint technique to build optimally basis functions based on all POD snapshots

- We want to build optimally goal-oriented basis functions *without computing/storing all the snapshots*?

RB + Greedy sampling strategy [Rozza, Huynh, Patera 2008]

Standard POD-Greedy algorithm

[Haasdonk *et al*. 2008] [Hoang *et al*. 2013]

(a) Set $Y_N^{\mathrm{st}} = 0$

(b) Set $\underline{\mu}_*^{\mathrm{st}} = \underline{\mu}_0$

(c) While $N \le N_{\max}^{\mathrm{st}}$

(d) $\mathcal{W}^{\mathrm{st}} = \left\{ \underline{e}_{\mathrm{proj}}^{\mathrm{st}}(\underline{\mu}_*^{\mathrm{st}}, t^k), 0 \le k \le K \right\}$

(e) $Y_{N+M}^{\mathrm{st}} \leftarrow Y_N^{\mathrm{st}} \bigoplus \mathrm{POD}(\mathcal{W}^{\mathrm{st}}, M)$

(f) $N \leftarrow N + M$

(g)
(h) $\underline{\mu}_*^{\mathrm{st}} = \arg \max_{\mu \in \Xi_{\mathrm{train}}} \left\{ \dfrac{\Delta_u(\underline{\mu})}{\sqrt{\sum_{k=1}^K \left\| \underline{u}_N^{\mathrm{st}}(\underline{\mu}, t^k) \right\|_Y^2}} \right\}$

(i) $S_*^{\mathrm{st}} \leftarrow S_*^{\mathrm{st}} \bigcup \left\{ \underline{\mu}_*^{\mathrm{st}} \right\}$

(j) end.

(k) $\Delta_u(\underline{\mu}) = \sqrt{\sum_{k=1}^K \left\| \underline{\mathcal{R}}^{\mathrm{st}}(\underline{v}; \underline{\mu}, t^k) \right\|_{Y'}^2}$

1) Where: given a set of snapshots $\{\underline{\xi}_k\}_{k=1}^{M_{\max}}$ the POD space W_M is defined as:

$$W_M = \arg \min_{V_M \subset \mathrm{span}\{\underline{\xi}_1, \ldots, \underline{\xi}_{M_{\max}}\}} \left(\frac{1}{M_{\max}} \sum_{k=1}^{M_{\max}} \inf_{\underline{\alpha}^k \in \mathbb{R}^M} \left\| \underline{\xi}_k - \sum_{m=1}^{M} \alpha_m^k \underline{v}_m \right\|^2 \right)$$

or, written as:

$$W_M = \mathrm{POD}\left(\{\underline{\xi}_1, \ldots, \underline{\xi}_{M_{\max}}\}, M \right)$$

2) Projection error:

$$\underline{e}_{\mathrm{proj}}^k(\underline{\mu}) = \underline{u}^k(\underline{\mu}) - \mathrm{proj}_{Y_N} \underline{u}^k(\underline{\mu})$$

3) Residual

$$\underline{\mathcal{R}}(\underline{v}; \underline{\mu}, t^k) = \underline{\mathcal{F}}(\underline{v}) - \underline{\underline{\mathcal{A}}}\left(\underline{u}_N^{k+1}(\underline{\mu}), \underline{v}; \underline{\mu} \right),$$
$$1 \le k \le K - 1$$

Goal-oriented vs. standard POD-Greedy algorithm

(a) Set $Y_N^{\mathrm{go}} = 0$

(b) Set $\underline{\mu}_*^{\mathrm{go}} = \underline{\mu}_0$

(c) While $N \le N_{\max}^{\mathrm{go}}$

(d) $\mathcal{W}^{\mathrm{go}} = \left\{ \underline{e}_{\mathrm{proj}}^{\mathrm{go}}(\underline{\mu}_*^{\mathrm{go}}, t^k), 0 \le k \le K \right\}$

(e) $Y_{N+M}^{\mathrm{go}} \leftarrow Y_N^{\mathrm{go}} \bigoplus \mathrm{POD}(\mathcal{W}^{\mathrm{go}}, M)$

(f) $N \leftarrow N + M$

CV process

(g) $\boxed{\begin{array}{l} \text{Find } \tilde{N} \text{ s.t. } \forall \underline{\mu} \in \Xi_n^{\mathrm{st}} \subset \Xi_{n+1}^{\mathrm{st}} \left(\subset S_*^{\mathrm{st}} \right) \\ \eta_T \le \left| \dfrac{\Delta_s(\underline{\mu})}{s(\underline{\mu}) - s_N^{\mathrm{go}}(\underline{\mu})} \right| \le 2 - \eta_T \end{array}}$

(h) $\underline{\mu}_*^{\mathrm{go}} = \arg \max_{\mu \in \Xi_{\mathrm{train}}} \left\{ \left| \dfrac{\Delta_s(\underline{\mu})}{s_{\tilde{N}}^{\mathrm{st}}(\underline{\mu})} \right| \right\}$

(i) $S_*^{\mathrm{go}} \leftarrow S_*^{\mathrm{go}} \bigcup \left\{ \underline{\mu}_*^{\mathrm{go}} \right\}$

(j) end.

Asymptotic output error estimation

(k) $\Delta_s(\underline{\mu}) = s_{\tilde{N}}^{\mathrm{st}}(\underline{\mu}) - s_N^{\mathrm{go}}(\underline{\mu})$

(a) Set $Y_N^{\mathrm{st}} = 0$

(b) Set $\underline{\mu}_*^{\mathrm{st}} = \underline{\mu}_0$

(c) While $N \le N_{\max}^{\mathrm{st}}$

(d) $\mathcal{W}^{\mathrm{st}} = \left\{ \underline{e}_{\mathrm{proj}}^{\mathrm{st}}(\underline{\mu}_*^{\mathrm{st}}, t^k), 0 \le k \le K \right\}$

(e) $Y_{N+M}^{\mathrm{st}} \leftarrow Y_N^{\mathrm{st}} \bigoplus \mathrm{POD}(\mathcal{W}^{\mathrm{st}}, M)$

(f) $N \leftarrow N + M$

(g)

(h) $\underline{\mu}_*^{\mathrm{st}} = \arg \max_{\mu \in \Xi_{\mathrm{train}}} \left\{ \dfrac{\Delta_u(\underline{\mu})}{\sqrt{\sum_{k=1}^{K} \left\| \underline{u}_N^{\mathrm{st}}(\underline{\mu}, t^k) \right\|_Y^2}} \right\}$

(i) $S_*^{\mathrm{st}} \leftarrow S_*^{\mathrm{st}} \bigcup \left\{ \underline{\mu}_*^{\mathrm{st}} \right\}$

(j) end.

(k) $\Delta_u(\underline{\mu}) = \sqrt{\sum_{k=1}^{K} \left\| \mathcal{R}^{\mathrm{st}}(\underline{v}; \underline{\mu}, t^k) \right\|_{Y'}^2}$

Cross-validation process

Algorithm 1 The "cross-validation" process.

INPUT: Ξ_n^{st}, N
OUTPUT: $\Xi_n^{\mathrm{st}}, \tilde{N}_n$

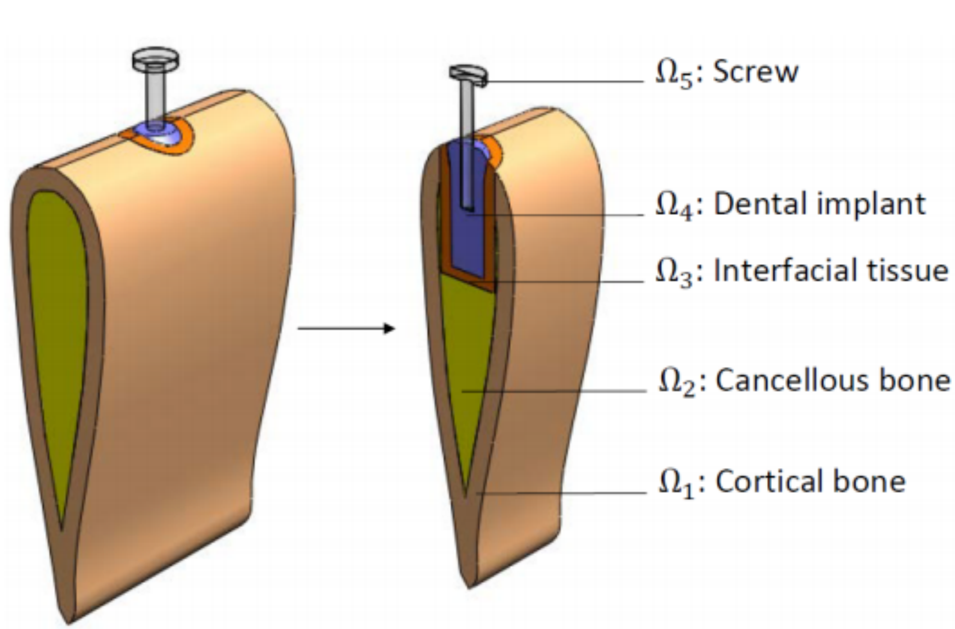
while true **do**
Given Ξ_n^{st};
Compute $\tilde{N}_n$ from this Ξ_n^{st}; (i.e., call the Algorithm 2 below)
Create Ξ_{n+1}^{st};
Check ($\clubsuit$) with $\tilde{N}_n$ over Ξ_{n+1}^{st}:
if ($\clubsuit$) holds $\forall \mu \in \Xi_{n+1}^{\mathrm{st}}$ **then** $\triangleright$ if ($\clubsuit$) holds
Get $\left\{\tilde{N}_n, \Xi_n^{\mathrm{st}}\right\}$;
Exit **while** loop;
else $\triangleright$ if ($\clubsuit$) is violated
$\Xi_n^{\mathrm{st}} \leftarrow \Xi_{n+1}^{\mathrm{st}}$;
end if
end while

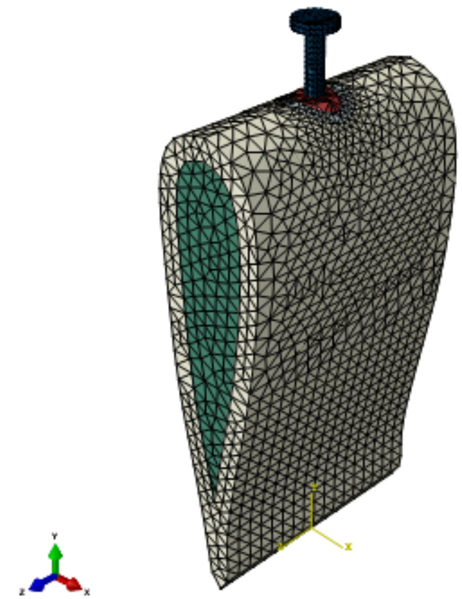
Algorithm 2 Function to compute $\tilde{N}$ based on input Ξ^{st} and N.

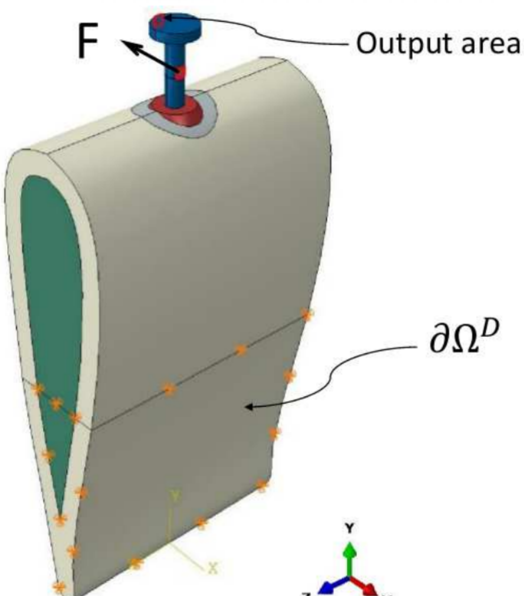
INPUT: Ξ^{st}, N
OUTPUT: $\tilde{N}$

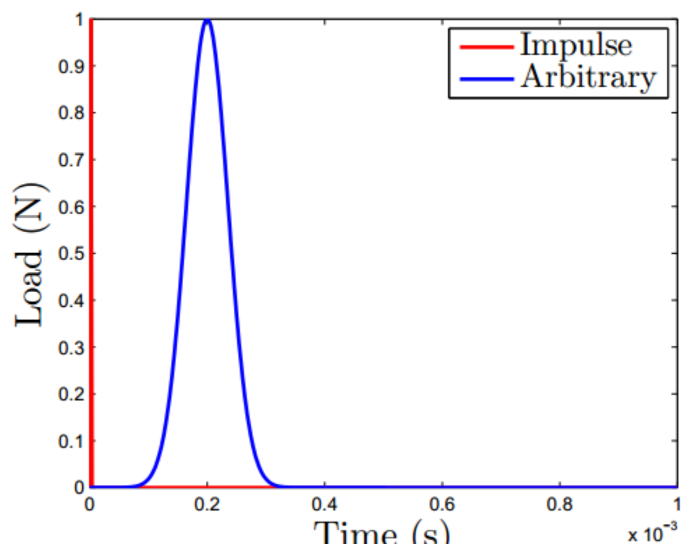
Start with $\tilde{N} = 2N$;
while true **do**
Check ($\clubsuit$) with $\tilde{N}$ over Ξ^{st}:
if any $\mu \in \Xi^{\mathrm{st}}$ violates ($\clubsuit$) **then** $\triangleright$ if ($\clubsuit$) is violated
if $\tilde{N} < N_{\mathrm{max}}^{\mathrm{st}}$ **then**
$\tilde{N} \leftarrow \tilde{N} + 1$;
else
Run the standard POD–Greedy algorithm to increase $N_{\mathrm{max}}^{\mathrm{st}}$: $N_{\mathrm{max}}^{\mathrm{st}} \leftarrow N_{\mathrm{max}}^{\mathrm{st}} + 1$;
end if
end if
if ($\clubsuit$) holds $\forall \mu \in \Xi^{\mathrm{st}}$ **then** $\triangleright$ if ($\clubsuit$) holds
Get $\tilde{N}$;
Exit **while** loop;
end if
end while

Numerical example: 3D dental implant model









$$\mathcal{N} = 26343$$

$$T = 0.001\text{s}$$

$$\Delta t = 2\times10^{-6}\text{s}$$

$$K = 500$$

$$\left|\Xi_{\text{train}}\right| = 900$$

3D Dental implant model problem...

- Material properties

Domain	Layers	E (Pa)	ν	$\rho(\mathrm{g/mm^3})$	β
Ω_1	Cortical bone	2.3162×10^{10}	0.371	1.8601×10^{-3}	3.38×10^{-6}
Ω_2	Cancellous bone	8.2345×10^{8}	0.3136	7.1195×10^{-4}	6.76×10^{-6}
Ω_3	Tissue	E	0.3155	1.055×10^{-3}	β
Ω_4	Titan implant	1.05×10^{11}	0.32	4.52×10^{-3}	5.1791×10^{-10}
Ω_5	Stainless steel screw	1.93×10^{11}	0.305	8.027×10^{-3}	2.5685×10^{-8}

$$\underline{\mu} = \left(E, \beta\right) \in \mathcal{D} \equiv [1\times10^6\mathrm{Pa}, 25\times10^6] \times [5\times10^{-6}, 5\times10^{-5}] \subset \mathbb{R}^{P=2}$$

- Explicit bi/linear forms:

$$f(v) = \sum_i \int_{\Gamma_1} v_i \bar{\phi}_i \, d\Gamma$$

$$m(w,v) = \sum_{r=1}^{5} \sum_i \int_{\Omega_r} \rho_r w_i v_i \, d\Omega$$

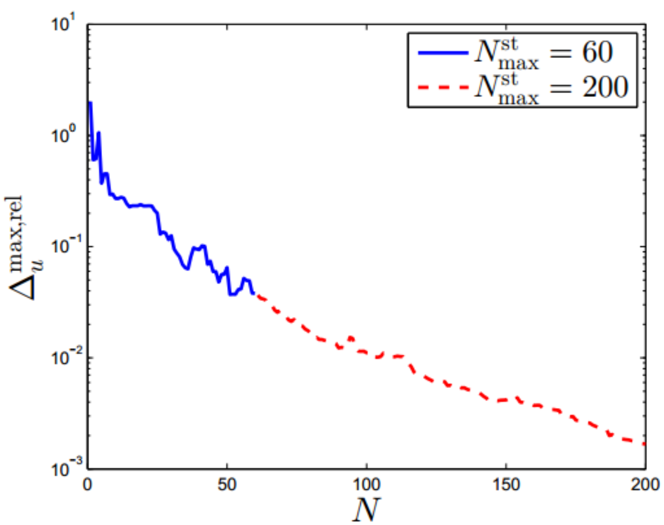
$$\ell(v) = \frac{1}{|\Gamma_o|} \int_{\Gamma_o} v_1 d\Gamma$$

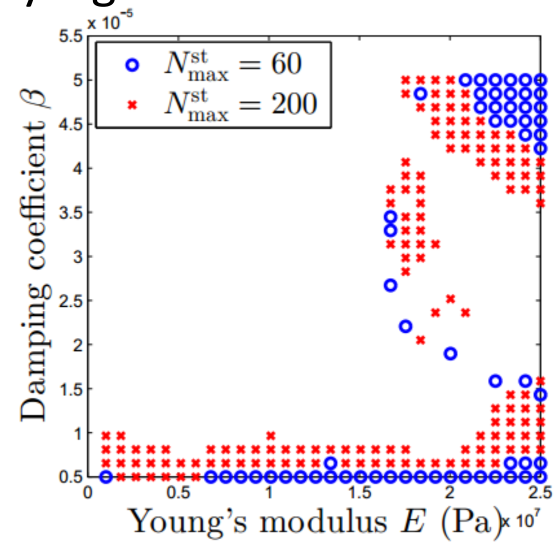
$$a(w,v;\mu) = \sum_{r=1, r\neq 3}^{5} \sum_{i,j,k,l} \int_{\Omega_r} \frac{\partial v_i}{\partial x_j} C^r_{ijkl} \frac{\partial w_k}{\partial x_l} d\Omega + \mu_1 \sum_{i,j,k,l} \int_{\Omega_3} \frac{\partial v_i}{\partial x_j} C^3_{ijkl} \frac{\partial w_k}{\partial x_l} d\Omega$$

$$c(w,v;\mu) = \sum_{r=1, r\neq 3}^{5} \beta_r \sum_{i,j,k,l} \int_{\Omega_r} \frac{\partial v_i}{\partial x_j} C^r_{ijkl} \frac{\partial w_k}{\partial x_l} d\Omega + \mu_2 \mu_1 \sum_{i,j,k,l} \int_{\Omega_3} \frac{\partial v_i}{\partial x_j} C^3_{ijkl} \frac{\partial w_k}{\partial x_l} d\Omega$$

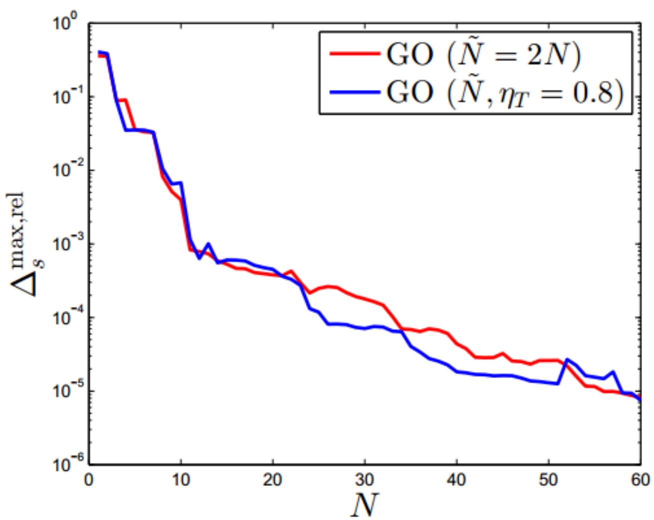
Numerical results…

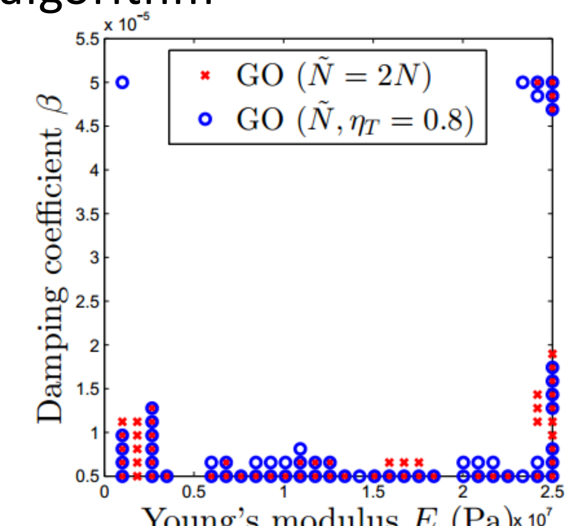
Standard POD-Greedy algorithm





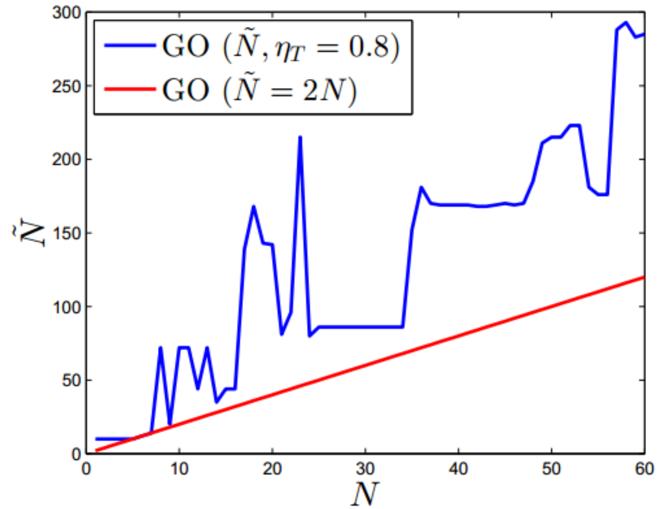
GO POD-Greedy algorithm

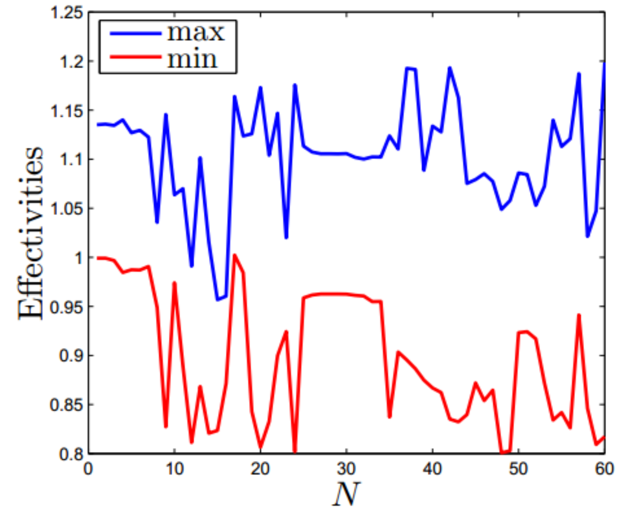




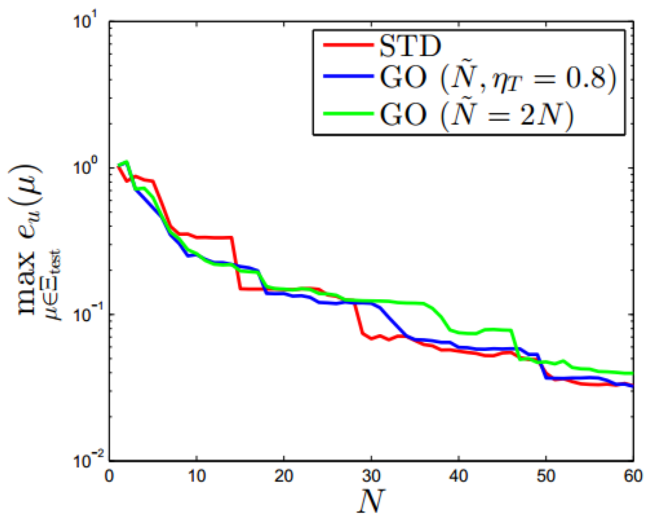
Numerical results…

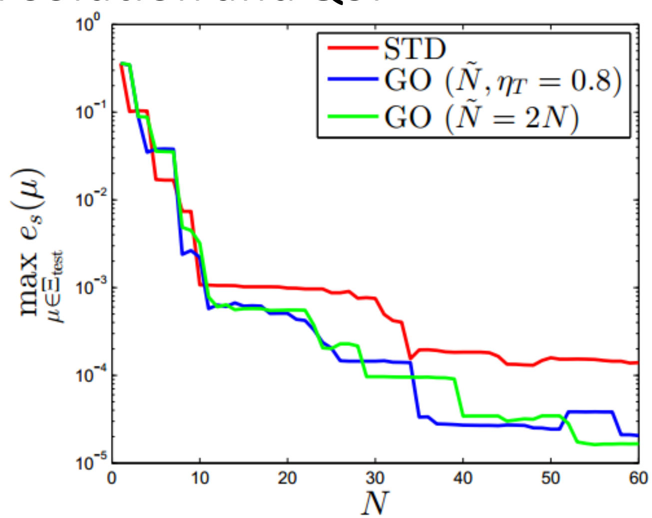
Cross-validation (CV) process





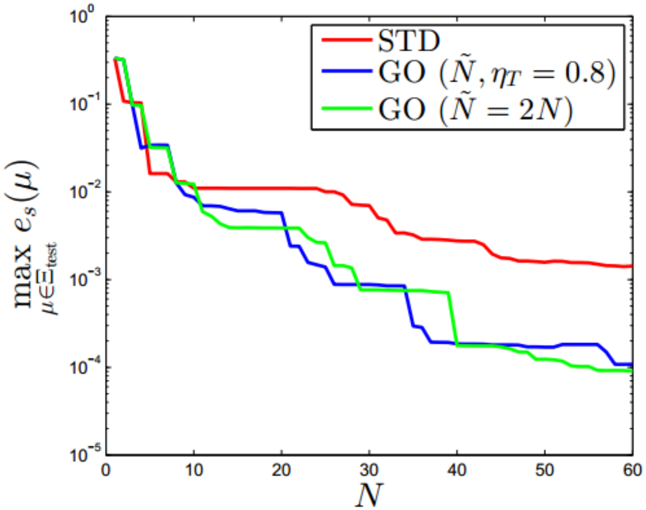
All true errors of solution and QoI

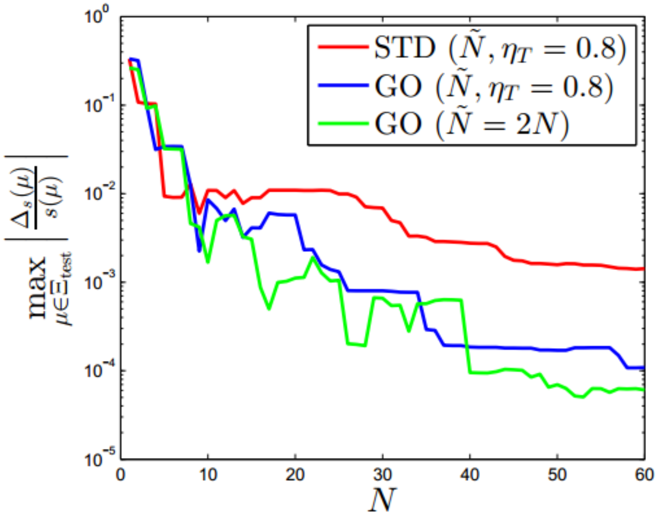




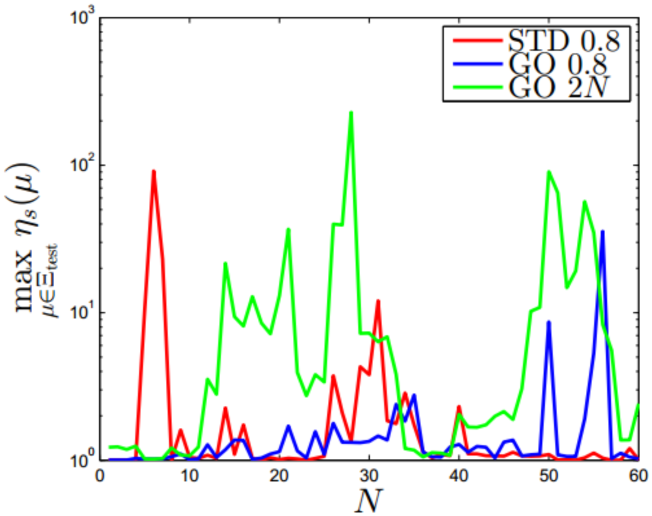
Numerical results: QoI

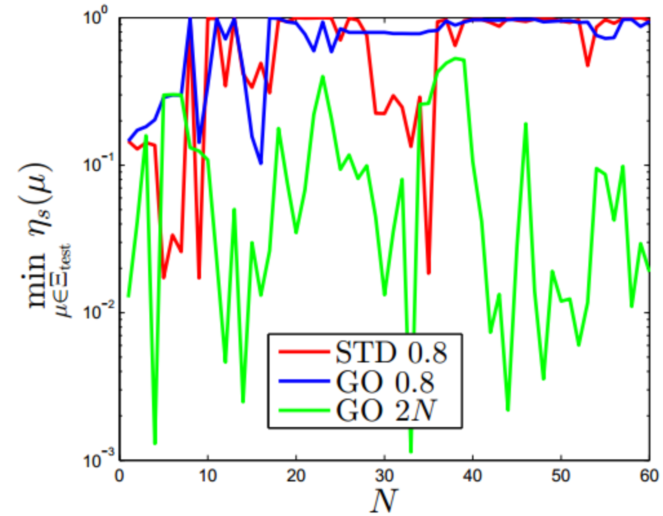
True errors vs Error approx. for case 1 Gauss load





Max and min effectivities for case 1 Gauss load





Numerical results…

- Computational time (online stage)

N	$t_{\mathrm{RB(online)}}$ (sec)	t_{FEM} (sec)	$\kappa = t_{\mathrm{FEM}}/t_{\mathrm{RB(online)}}$	$t_{\Delta_s(\mu)}$ (sec) $(\tilde{N} = 2N)$	$t_{\Delta_s(\mu)}$ (sec) $(\tilde{N}, \eta_T = 0.8)$
10	0.006757	29	4291	0.008329	0.038035
20	0.008391	29	3456	0.014242	0.099046
30	0.011123	29	2607	0.031723	0.049015
40	0.014531	29	1996	0.042440	0.130987
50	0.024381	29	1189	0.061122	0.192829
60	0.031196	29	930	0.075049	0.328012

- All calculations were performed on a desktop *Intel(R) Core(TM) i7-3930K CPU @3.20GHz 3.20GHz, RAM 32GB , 64-bit Operating System*.

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