Space-time goal-oriented reduced basis approximation for linear wave equation

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Outline

1. Motivation
   - Linear Wave Equation
   - Finite Element Approximation
   - Reduced Basis Approximation
   - (Standard) POD-Greedy Sampling Strategy

2. Proposed Algorithm
   - Goal-oriented (GO) POD-Greedy Sampling Strategy

3. Numerical Example
   - 3D Dental Implant Model Problem

4. Conclusion

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Problem statement: strong form

- Consider a spatial domain $\Omega \in \mathbb{R}^d$, Lipschitz continuous boundary Γ
- Dynamic linear elasticity equilibrium (assume Rayleigh damping):

$$\frac{\partial \sigma_{ij}^e}{\partial x_j} + b_i = \rho \frac{\partial^2 u_i^e}{\partial t^2} + \alpha(\mu)\rho \frac{\partial u_i^e}{\partial t}$$

- Constitutive relations (homogeneous, isotropic materials)

$$\sigma_{ij}^e = C_{ijkl}(\mu)\left(\frac{\partial u_k^e}{\partial x_l} + \beta(\mu) \frac{\partial}{\partial t} \frac{\partial u_k^e}{\partial x_l} \right)$$

- Initial conditions: $u_i^e(x,0) = 0$ and $\frac{\partial u_i^e}{\partial t}(x,0) = 0$
- Boundary conditions: $u_i^e = 0$ on Γ_D; surface traction $\sigma_{ij}^e \hat{n}_j = \mathrm{t}_i$ on Γ_N

Problem statement: weak form

- In space setting:

$$\int_\Omega \rho v_i \frac{\partial^2 u_i^e}{\partial t^2} + \int_\Omega \alpha(\mu)\rho v_i \frac{\partial u_i^e}{\partial t} + \beta(\mu)\frac{\partial}{\partial t}\int_\Omega \frac{\partial v_i}{\partial x_j} C_{ijkl}(\mu)\frac{\partial u_k^e}{\partial x_l}$$
$$+\int_\Omega \frac{\partial v_i}{\partial x_j} C_{ijkl}(\mu)\frac{\partial u_k^e}{\partial x_l} = \int_\Omega b_i v_i + \int_{\Gamma_N} v_i \mathsf{t}_i, \quad \forall v \in Y^e, \mu \in \mathcal{D}$$

- Or, equivalently:

$$m\left(\frac{\partial^2 u^e}{\partial t^2}, v\right) + c\left(\frac{\partial u^e}{\partial t}, v; \mu\right) + a(u^e, v; \mu) = f(v), \quad \forall v \in Y^e, \mu \in \mathcal{D}$$

- Space-time quantity of interest:

$$\mu\left(\rightarrow u^e(\mu)\right) \rightarrow s^e(\mu)?$$

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

Finite element discretization

Trapezoidal rule

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

$$\boxed{\mathcal{A}\Big(u^{k+1}(\mu), v; \mu\Big) = \mathcal{F}(v),} \qquad \forall v \in Y, \mu \in \mathcal{D}, \quad 1 \leq k \leq K-1$$

$$\begin{cases} \mathcal{A}\Big(u^{k+1}(\mu), v; \mu\Big) = \dfrac{1}{\Delta t^2} m(u^{k+1}(\mu), v; \mu) + \dfrac{1}{2\Delta t} c(u^{k+1}(\mu), v; \mu) + \dfrac{1}{4} a(u^{k+1}(\mu), v; \mu) \\ \mathcal{F}(v) = -\dfrac{1}{\Delta t^2} m(u^{k-1}(\mu), v; \mu) + \dfrac{1}{2\Delta t} c(u^{k-1}(\mu), v; \mu) - \dfrac{1}{4} a(u^{k-1}(\mu), v; \mu) \\ \qquad + \dfrac{2}{\Delta t^2} m(u^{k}(\mu), v; \mu) - \dfrac{1}{2} a(u^{k}(\mu), v; \mu) + g^{eq}(t^k) f(v; \mu) \\ u(\mu, t^0) = 0, \quad \dfrac{\partial u(\mu, t^0)}{\partial t} = 0 \end{cases}$$

$$\boxed{\mu \Big(\rightarrow u(\mu)\Big) \rightarrow s(\mu)?}$$

  - FE quantity of interest:

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

Reduced-order approximation: Galerkin projection

- Introduce $S_* = \{\mu_1 \in \mathcal{D}, \mu_2 \in \mathcal{D}, \ldots, \mu_N \in \mathcal{D}\}, 1 \le N \le N_{\max}$; and nested Lagrangian RO spaces $Y_N = \mathrm{span}\{\zeta_n, 1 \le n \le N\}, 1 \le N \le N_{\max}$

  - Galerkin projection:

$$u_N(\mu, t^k) = \sum_{n=1}^{N} u_{N\,n}(\mu, t^k)\,\zeta_n, \quad \forall \zeta_n \in Y_N,\ 1 \le k \le K$$

  - Solve the following elliptic systems

$$\boxed{\mathcal{A}\left(u_N^{k+1}(\mu), v; \mu\right) = \mathcal{F}(v),} \ \forall v \in Y_N, \mu \in D,\ 1 \le k \le K-1$$

$$\boxed{\mu\left(\to u_N(\mu)\right) \to s_N(\mu)?}$$

  - RO quantity of interest:

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

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 a dual/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 $\mu_*^{\mathrm{st}} = \mu_0$

(c) While $N \leq N_{\max}$

(d) $\mathcal{W}^{\mathrm{st}} = \left\{ e_{\mathrm{proj}}^{\mathrm{st}}(\mu_*^{\mathrm{st}}, t^k), 0 \leq k \leq K \right\}$

(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) $\mu_*^{\mathrm{st}} = \arg \max\limits_{\mu \in \Xi_{\mathrm{train}}} \left\{ \Delta_u(\mu) \right\}$

(h) $S_*^{\mathrm{st}} \leftarrow S_*^{\mathrm{st}} \bigcup \left\{ \mu_*^{\mathrm{st}} \right\}$

(i) end.

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

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

$$W_M = \arg \min_{V_M \subset \mathrm{span}\{\xi_1, \ldots, \xi_{M_{\max}}\}} \left(\frac{1}{M_{\max}} \sum_{k=1}^{M_{\max}} \inf_{\underline{\alpha}^k \in \mathbb{R}^M} \left\| \xi_k - \sum_{m=1}^{M} \alpha_m^k v_m \right\|^2 \right)$$

or, written as:

$$W_M = \mathrm{POD}\left(\{\xi_1, \ldots, \xi_{M_{\max}}\}, M \right)$$

2) Projection error:

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

3) Residual

$$\mathcal{R}(v; \mu, t^k) = \mathcal{F}(v) - \mathcal{A}\left(u_N^{k+1}(\mu), v; \mu \right)$$

$$1 \leq k \leq K - 1$$

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Goal-oriented POD-Greedy algorithm

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

(b) Set $\mu_*^{\text{st}} = \mu_0$

(c) While $N \leq N_{\max}$

(d) $\mathcal{W}^{\text{st}} = \left\{ e_{\text{proj}}^{\text{st}}(\mu_*^{\text{st}}, t^k), 0 \leq k \leq K \right\}$

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

(f) $N \leftarrow N + M$

(g) $\mu_*^{\text{st}} = \arg \max_{\mu \in \Xi_{\text{train}}} \left\{ \Delta_u(\mu) \right\}$

(h) $S_*^{\text{st}} \leftarrow S_*^{\text{st}} \bigcup \left\{ \mu_*^{\text{st}} \right\}$

(i) end.

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

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

(b) Set $\mu_*^{\text{go}} = \mu_0$

(c) While $N \leq N_{\max}$

(d) $\mathcal{W}^{\text{go}} = \left\{ e_{\text{proj}}^{\text{go}}(\mu_*^{\text{go}}, t^k), 0 \leq k \leq K \right\}$

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

(f) $N \leftarrow N + M$

(g) $\mu_*^{\text{go}} = \arg \max_{\mu \in \Xi_{\text{train}}} \left\{ \Delta_s(\mu) \right\}$ ← NEW

(h) $S_*^{\text{go}} \leftarrow S_*^{\text{go}} \bigcup \left\{ \mu_*^{\text{go}} \right\}$

(i) end.

(j) $$\Delta_s(\mu) = \left| \frac{s_{2N}^{\text{st}}(\mu) - s_N^{\text{go}}(\mu)}{s_{2N}^{\text{st}}(\mu)} \right|$$

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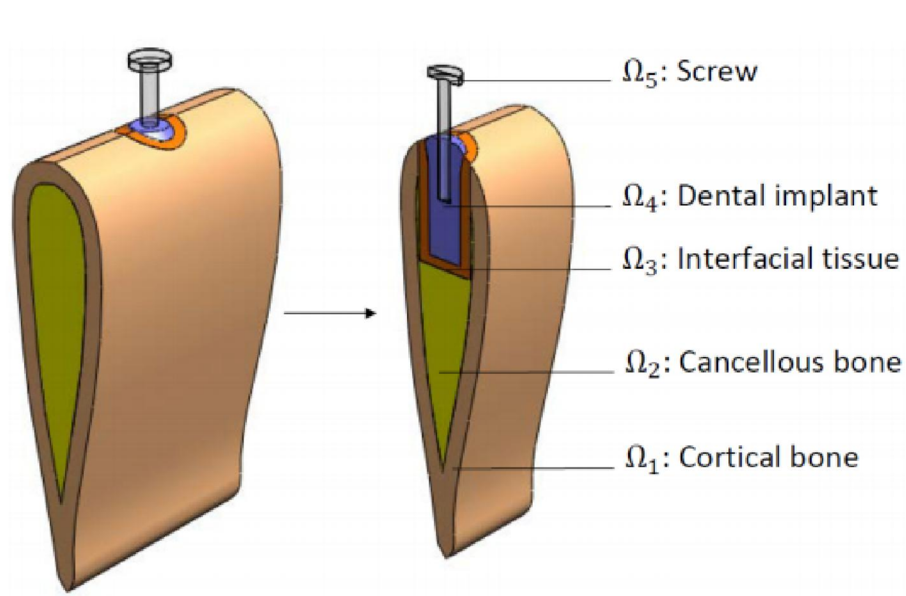
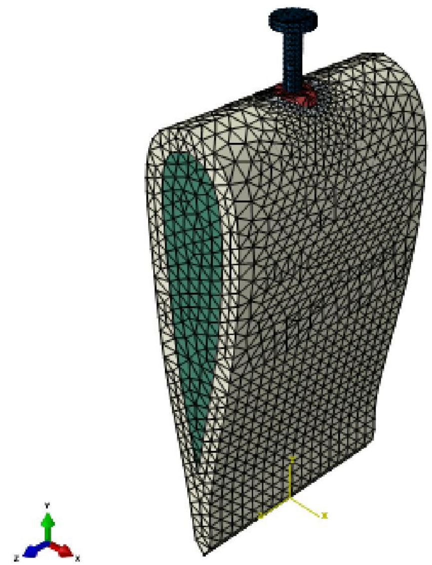
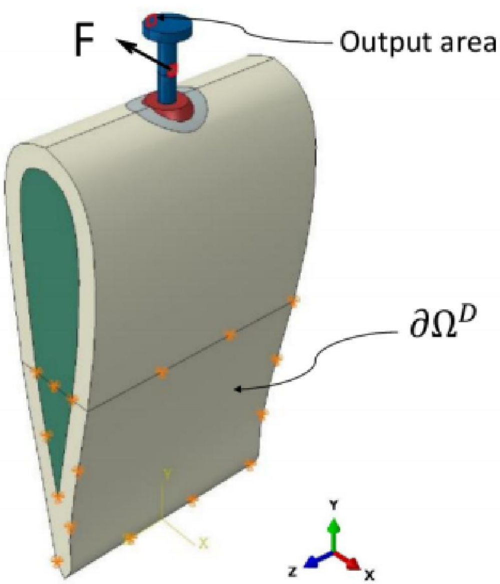
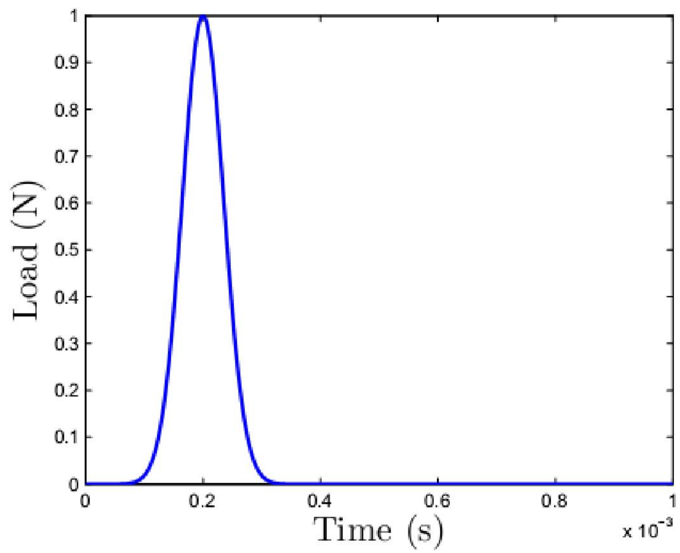
3D Dental implant model problem









Example; in practice, use Dirac Delta loading with Duhamel's principle.

3D Dental implant model problem (cont.)

- 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}

- Explicit bi/linear forms:

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

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

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

$$f(v) = \int_{\Gamma_1} v$$

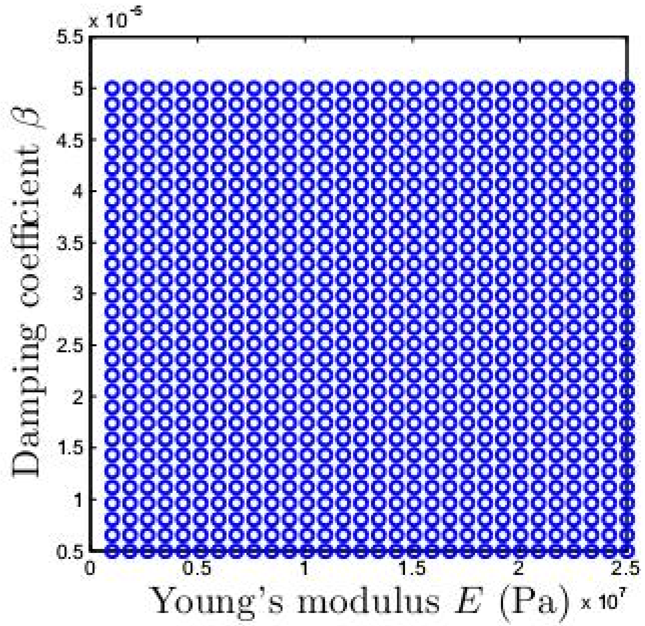
$$\ell(v) = \frac{1}{|\Gamma_o|} \int_{\Gamma_o} v$$

Numerical results

- FE dof: $\mathcal{N} = 26343$
- Time integration: $T = 1 \times 10^{-3}\mathrm{s}$, $\Delta t = 2 \times 10^{-6}\mathrm{s}$, $K = \dfrac{T}{\Delta t} = 500$
- Parameter domain:

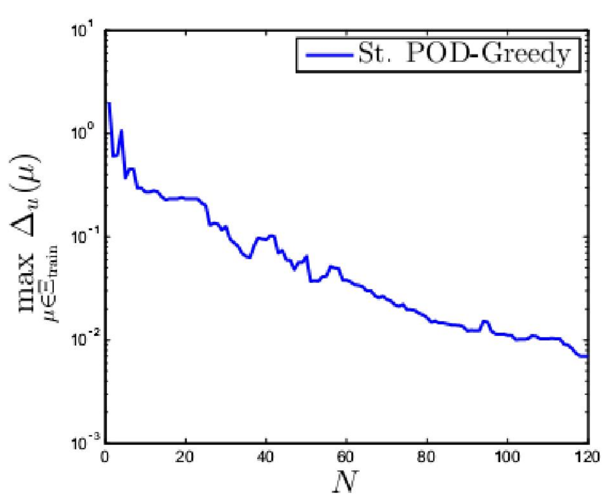
$$\mathcal{D} \equiv [1 \times 10^6, 25 \times 10^6]\mathrm{Pa} \times [5 \times 10^{-6}, 5 \times 10^{-5}] \subset \mathbb{R}^{P=2}$$

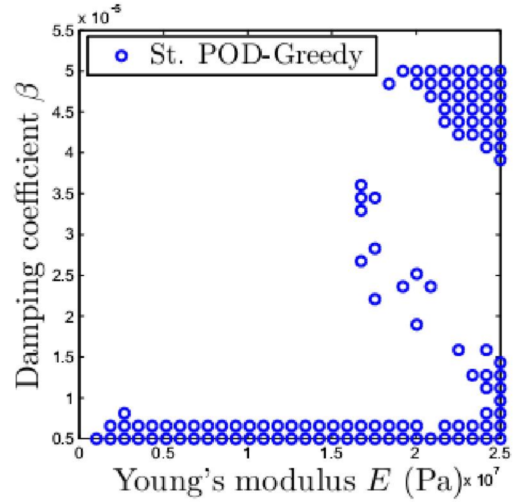
- Training sample set: $n_{\mathrm{train}} = 900$

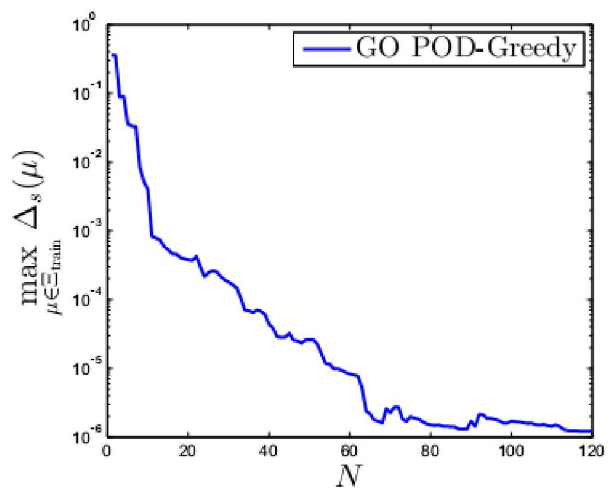


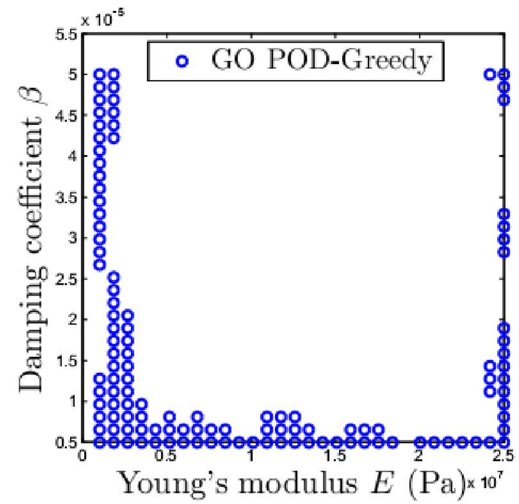
Numerical results (cont.)

- Offline stages of Std vs. GO POD-Greedy algorithms









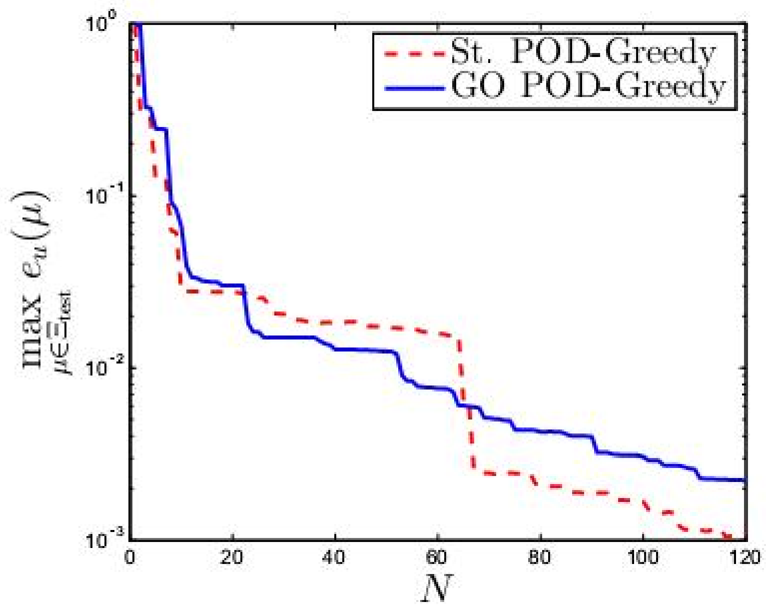
True error comparison (validation)

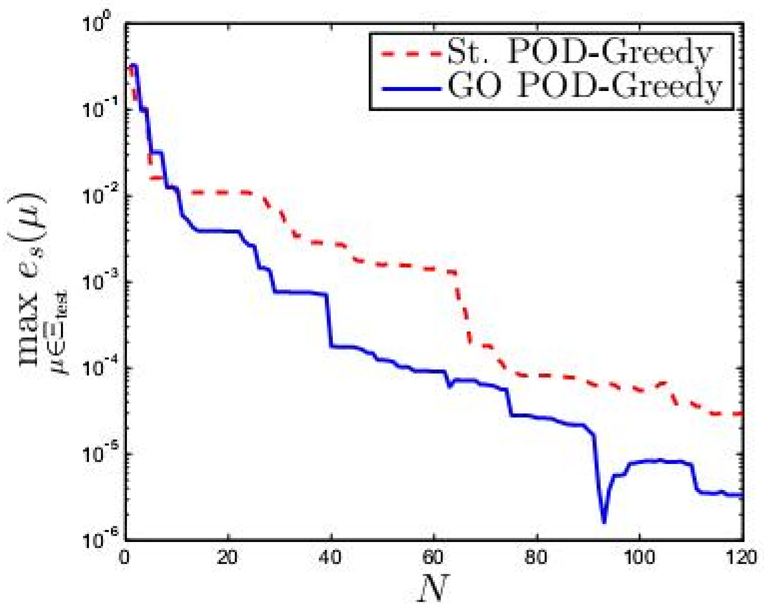
$$e_u^{\text{st}}(\mu) = \frac{\sum_{k=0}^{K-1} \int_{t^k}^{t^{k+1}} \left\| u(\mu,t) - u_N^{\text{st}}(\mu,t) \right\|_Y dt}{\sum_{k=0}^{K-1} \int_{t^k}^{t^{k+1}} \left\| u(\mu,t) \right\|_Y dt}$$

$$e_s^{\text{st}}(\mu) = \left| \frac{s(\mu) - s_N^{\text{st}}(\mu)}{s(\mu)} \right|$$

$$e_u^{\text{go}}(\mu) = \frac{\sum_{k=0}^{K-1} \int_{t^k}^{t^{k+1}} \left\| u(\mu,t) - u_N^{\text{go}}(\mu,t) \right\|_Y dt}{\sum_{k=0}^{K-1} \int_{t^k}^{t^{k+1}} \left\| u(\mu,t) \right\|_Y dt}$$

$$e_s^{\text{go}}(\mu) = \left| \frac{s(\mu) - s_N^{\text{go}}(\mu)}{s(\mu)} \right|$$





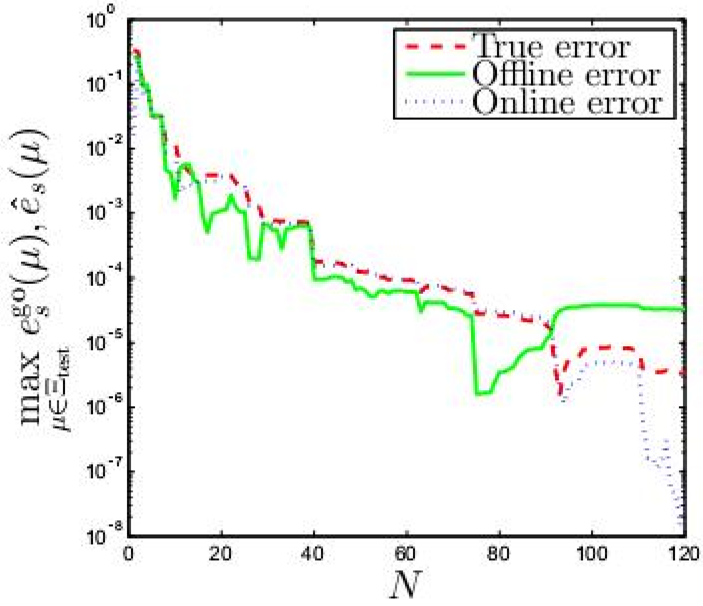
GO algorithm: error estimate

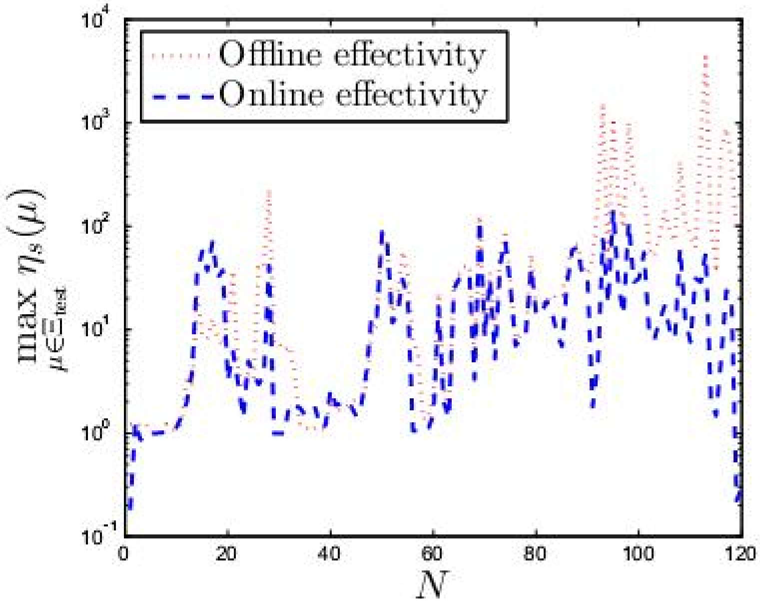
$$\hat{e}_s^{\mathrm{off}}(\mu) = \left| \frac{s_{2N}^{\mathrm{st}}(\mu) - s_N^{\mathrm{go}}(\mu)}{s(\mu)} \right|$$

$$\eta_s^{\mathrm{off}}(\mu) = \left| \frac{s_{2N}^{\mathrm{st}}(\mu) - s_N^{\mathrm{go}}(\mu)}{s(\mu) - s_N^{\mathrm{go}}(\mu)} \right|$$

$$\hat{e}_s^{\mathrm{onl}}(\mu) = \left| \frac{s_{2N}^{\mathrm{go}}(\mu) - s_N^{\mathrm{go}}(\mu)}{s(\mu)} \right|$$

$$\eta_s^{\mathrm{onl}}(\mu) = \left| \frac{s_{2N}^{\mathrm{go}}(\mu) - s_N^{\mathrm{go}}(\mu)}{s(\mu) - s_N^{\mathrm{go}}(\mu)} \right|$$





Computational time

- Computational time:

N	$t_{RB(online)}$ (sec)	t_{FEM} (sec)	$\kappa = t_{FEM}/t_{RB(online)}$
10	0.0072	29	4027
20	0.0081	29	3580
30	0.0106	29	2736
40	0.0140	29	2070
50	0.0243	29	1193
60	0.0300	29	966

- All calculations were performed on a desktop *Intel(R) Core(TM) i7-3930K CPU @3.20GHz 3.20GHz, RAM 32GB , 64-bit Operating System*.
- The work focuses on real-time context with many online computations, the offline stage is done once and expensive: the total computational time is approximately 2 weeks (including all FEM solutions/outputs and RB true errors of the standard and goal-oriented algorithms) on this computer.

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Conclusions

- A new algorithm is proposed based on a *novel idea*: build optimally goal-oriented basis functions *without computing/storing all the snapshots*.
- The proposed algorithm still needs the standard POD-Greedy algorithm as it provides an *error estimate* for the quantity of interest.
- Simple, easy to implement; same computational cost.
- Applicable to any regular output functional; it *cooperates and improve* further the standard algorithm.

Sponsors

European Research Council Starting Independent Research Grant (ERC Stg grant agreement No. 279578) entitled *"Towards real time multiscale simulation of cutting in non-linear materials with applications to surgical simulation and computer guided surgery"*.

Thank you for your attention!

Khac Chi Hoang, Pierre Kerfriden, Stephane PA Bordas, *Space-time goal-oriented reduced basis approximation for linear wave equation*, arXiv:1305.3528

Questions?