Non-intrusive data-driven structural optimization with ROMs and parameter space reduction

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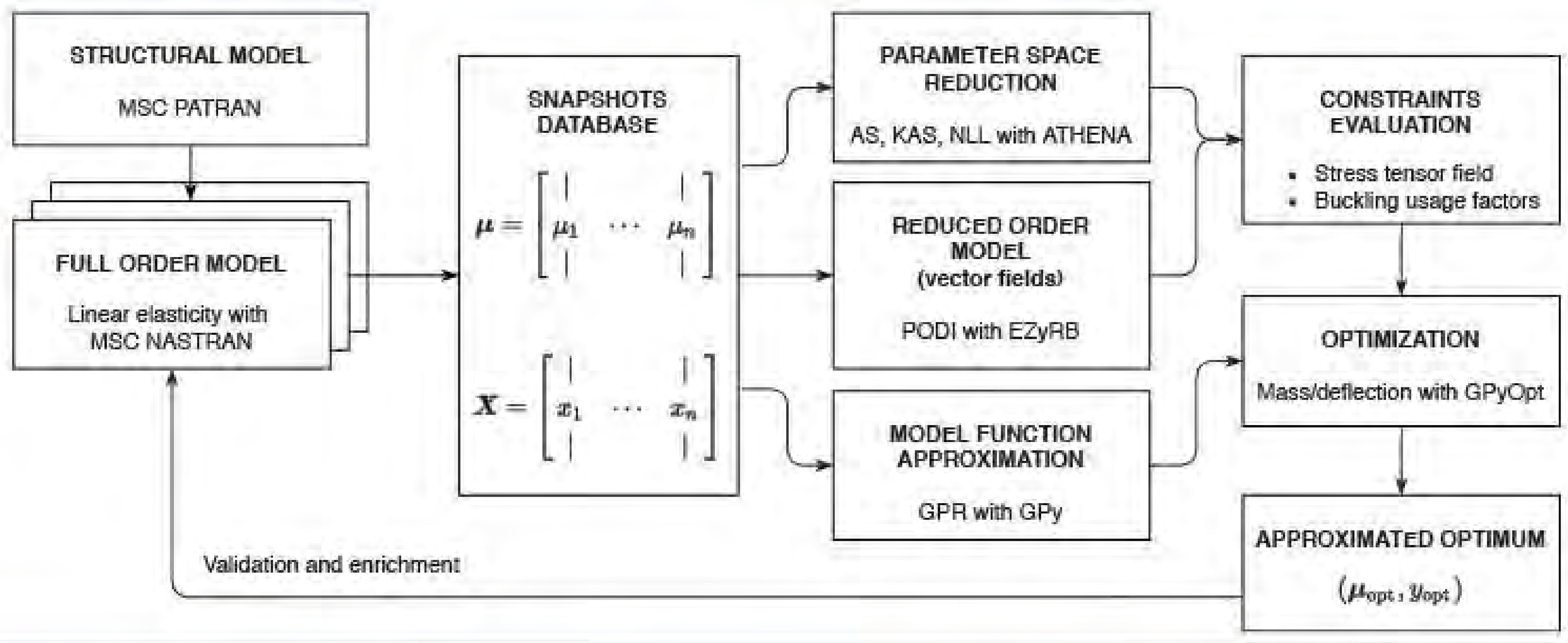
Structural optimization pipeline based on Reduced Order Methods (ROMs)

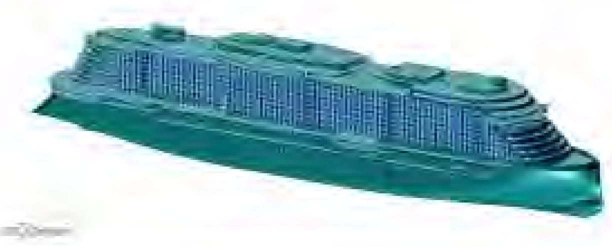
We present a structural optimization computational pipeline. We exploit **MSC Patran** and **MSC Nastran** softwares to create a solutions database for different input parameters. Then we apply non-intrusive Reduced Order Methods (ROMs) such as **Proper Orthogonal Decomposition with Interpolation (PODI)** to predict the solution fields of interest, and **Active Subspaces (AS)** to reduce the parameter space dimensionality and perform sensitivity analysis over the parameters, using open source Python packages.
Finally Bayesian optimization is employed to minimize a target scalar function while ROMs serve as enablers for fast and accurate real-time evaluations.

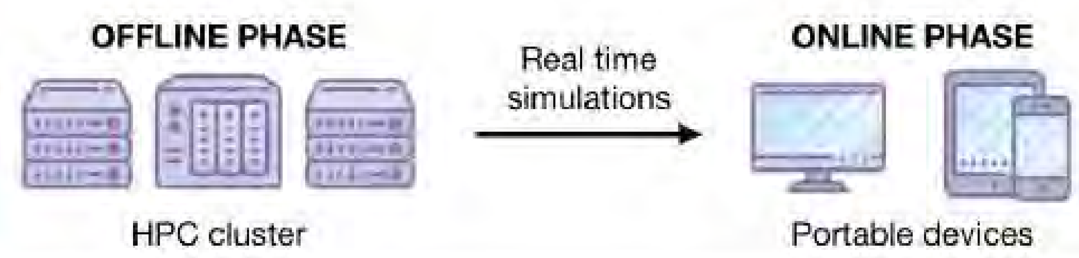


1 - Proper Orthogonal Decomposition with Interpolation (PODI) [3]

POD with interpolation main features:

- No need to know the underlying equations/matrices (as for POD-Galerkin method).
- SVD of the snapshots matrix $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^*$.
- Using the first N modes $\mathbf{U}_N$, we are able to span the low-dimensional space on which we project the original samples.
- The **modal coefficients** are computed as $\mathbf{C} = \mathbf{U}_N^T\mathbf{X}$.
- Real-time computation of the solution fields for any new parameter by interpolating the modal coefficients
- **Offline-online paradigm** allows to efficiently exploit all the collected simulations to make **real-time predictions** (moreover we can enrich the database!)





2 - Active Subspaces (AS) [1, 2]

Consider a function, its gradient vector, and a sampling p.d.f.

$$f = f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^m, \quad \nabla f(\mathbf{x}) \in \mathbb{R}^m, \quad \rho : \mathbb{R}^m \to \mathbb{R}_+$$

Take the average outer product of the gradients and partition its eigendecomposition,

$$\mathbf{C} = \mathbb{E}[\nabla_\mathbf{x} f \, \nabla_\mathbf{x} f^T] = \int (\nabla_\mathbf{x} f)(\nabla_\mathbf{x} f)^T \rho \, d\mathbf{x} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$$

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & \\ & \mathbf{\Lambda}_2 \end{bmatrix}, \qquad \mathbf{W} = [\mathbf{W}_1 \quad \mathbf{W}_2], \qquad \mathbf{W}_1 \in \mathbb{R}^{m \times n}$$

Rotate and separate the coordinates:

$$\mathbf{x} = \mathbf{W}\mathbf{W}^T\mathbf{x} = \mathbf{W}_1\mathbf{W}_1^T\mathbf{x} + \mathbf{W}_2\mathbf{W}_2^T\mathbf{x} = \mathbf{W}_1\mathbf{y} + \mathbf{W}_2\mathbf{z}$$

We call $\mathbf{y}$ the **active variable** and $\mathbf{z}$ the inactive one:

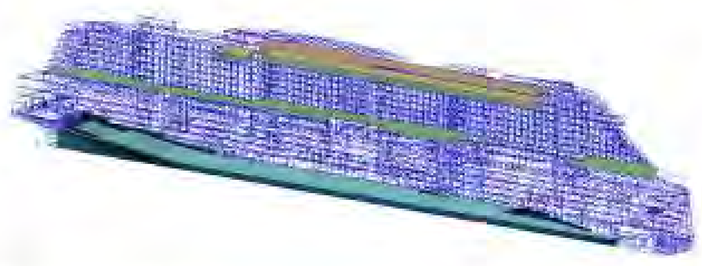
$$\mathbf{y} = \mathbf{W}_1^T\mathbf{x} \in \mathbb{R}^n, \qquad \mathbf{z} = \mathbf{W}_2^T\mathbf{x} \in \mathbb{R}^{m-n}$$

github.com/mathLab/ATHENA

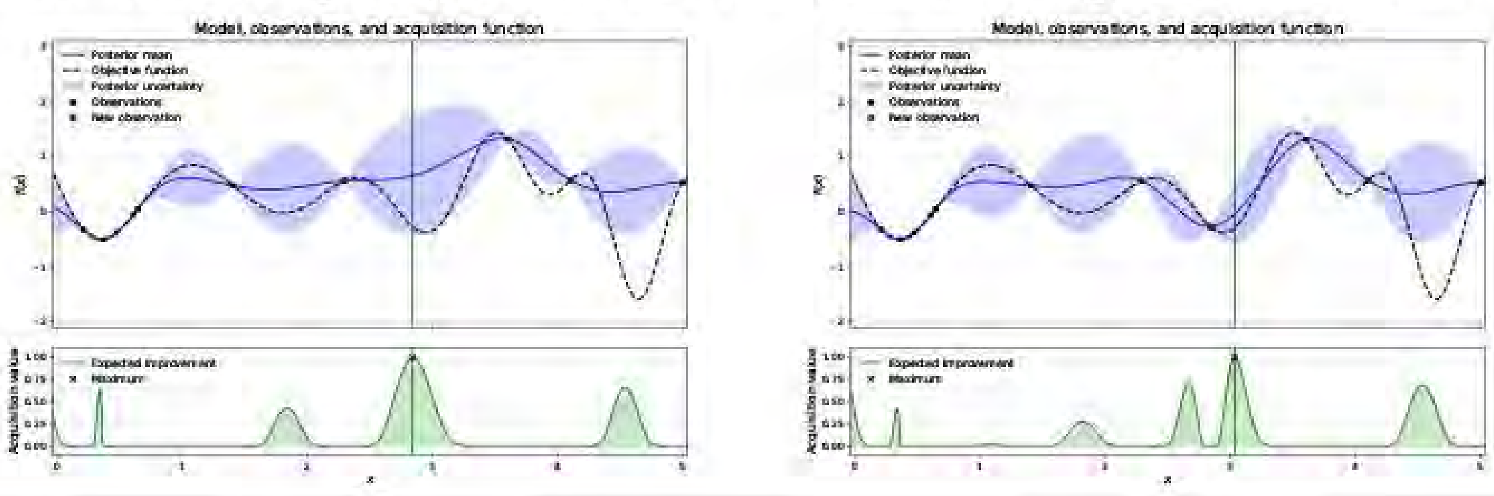
3 - Bayesian optimization

We seek a global minimizer of an unknown function of interest using a Bayesian optimization approach

$$x_{\text{opt}} = \arg\min_{\mathbf{x} \in \Omega} f(\mathbf{x})$$

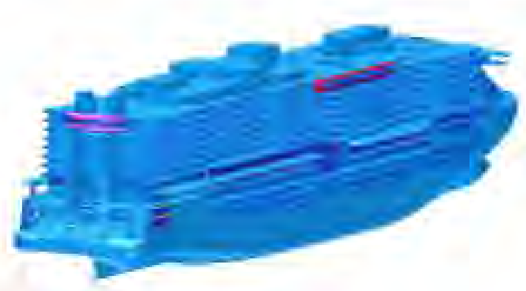


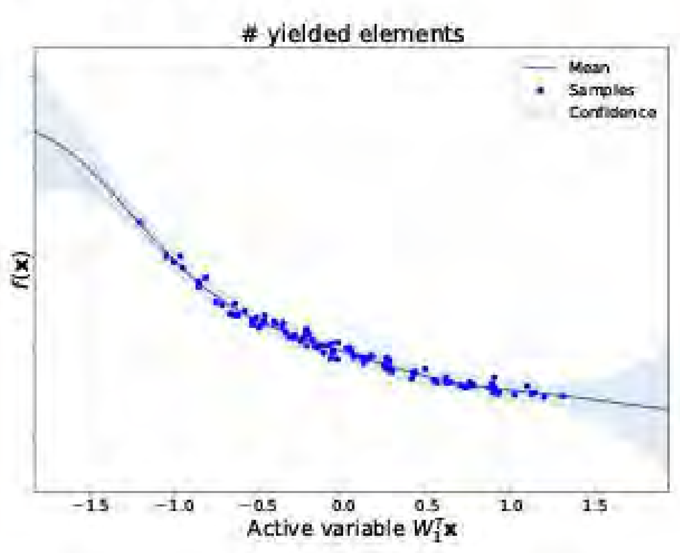
We maximize the **Expected Improvement** acquisition function, depicted in green below with an illustrative example, to select the next sample to evaluate. Our design inputs are the thickness of 6 regions of the hull.

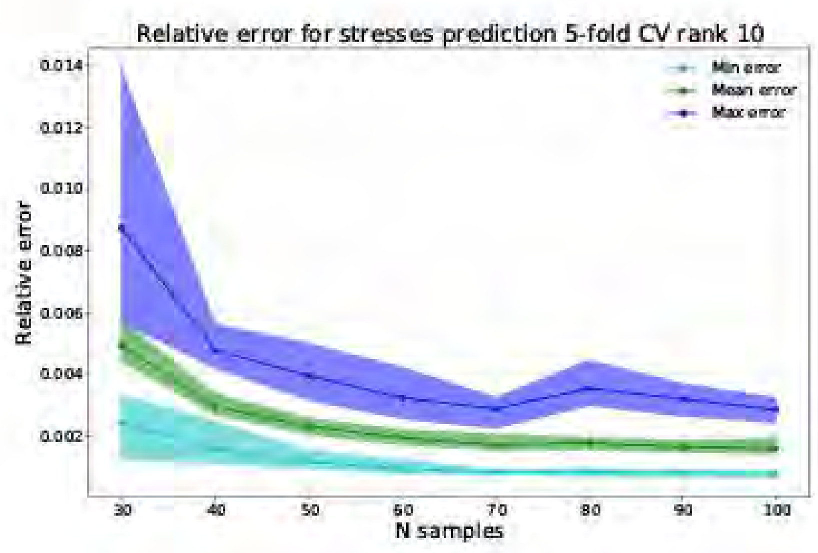


4 - Solution fields and constraints prediction

Using PODI we predict the stress tensor field for new parameters with an L^2 relative error smaller than 0.3%. Costraints such as the **number of yielded or buckled elements** are evaluated thorugh **GP regression** over the active subspace.

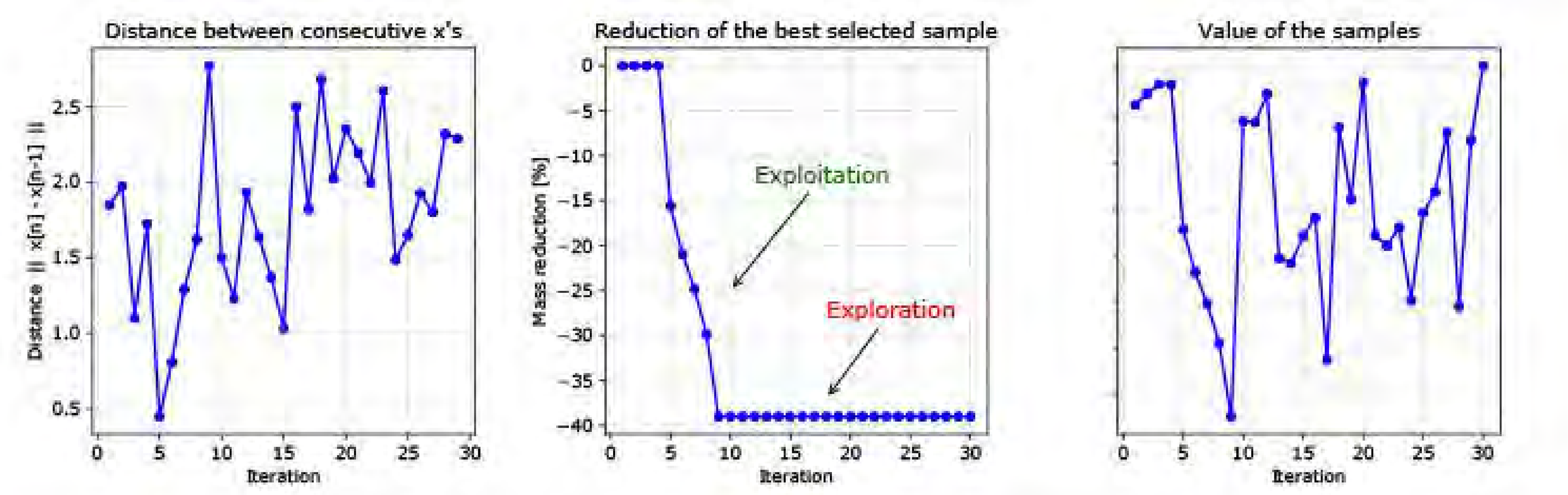






5 - Numerical results

We minimize the mass of the parametrized decks of the hull, under the constraints of a prescribed maximum number of yielded and buckled elements, for a given load condition. We achieve very good results.
ROMs are used to reconstruct the stress tensor and the buckling usage factors fields for new untried parameters in real-time. AS is employed to reduce the number of parameters for the constraints evaluation.



References and Acknowledgements

[1] P. G. Constantine. *Active subspaces: Emerging ideas for dimension reduction in parameter studies*, volume 2 of *SIAM Spotlights*. SIAM, 2015.

[2] N. Demo, M. Tezzele, and G. Rozza. A non-intrusive approach for reconstruction of POD modal coefficients through active subspaces. *Comptes Rendus Mécanique de l'Académie des Sciences, DataBEST 2019 Special Issue*, 347(11):873–881, November 2019.

[3] M. Tezzele, N. Demo, A. Mola, and G. Rozza. An integrated data-driven computational pipeline with model order reduction for industrial and applied mathematics. *Special Volume ECMI, In Press*, 2020.

This work was partially supported by an industrial Ph.D. grant sponsored by Fincantieri S.p.A., and by European Union Funding for Research and Innovation — Horizon 2020 Program — in the framework of European Research Council Executive Agency: H2020 ERC CoG 2015 AROMA-CFD project 681447 "Advanced Reduced Order Methods with Applications in Computational Fluid Dynamics" P.I. Professor Gianluigi Rozza. We also gratefully thank Ing. Matteo Sidari and Ing. Mauro Sicchiero for their precious comments and suggestions.