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

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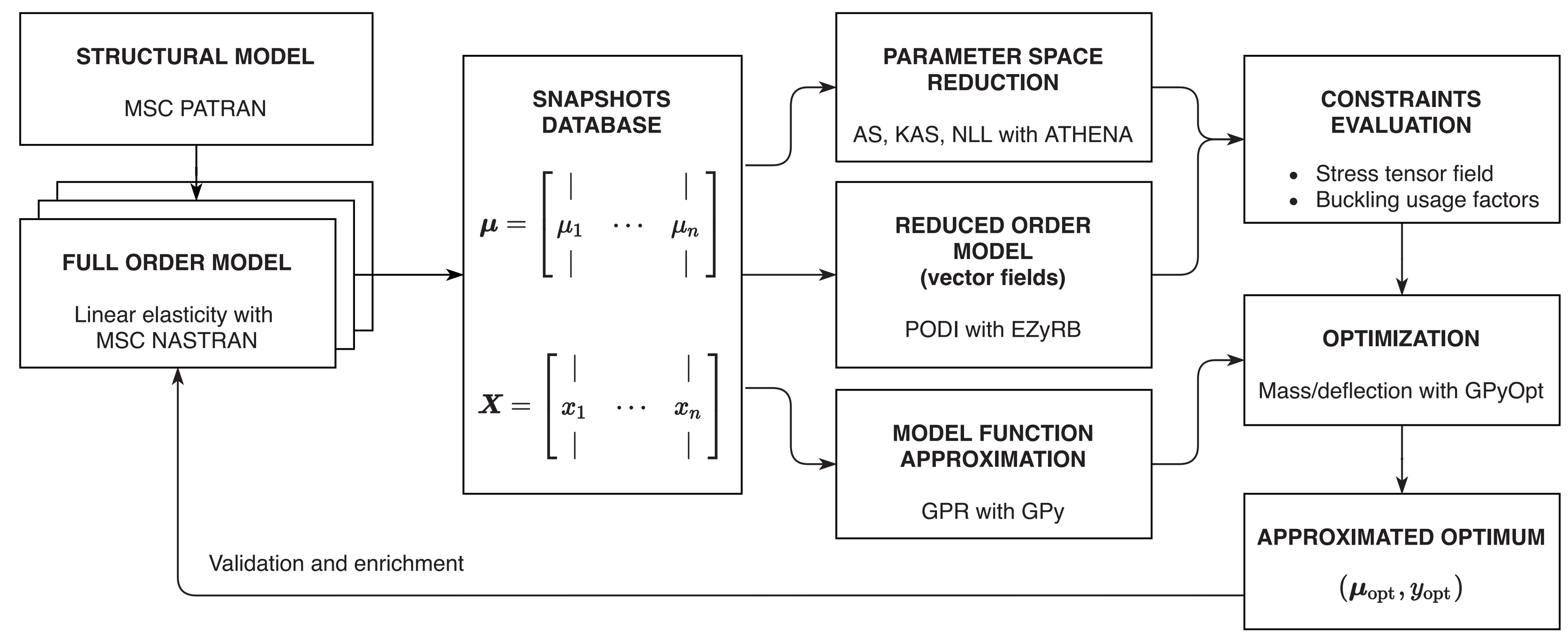
Structural optimization pipeline based on Reduced Order Methods (ROMs)

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.

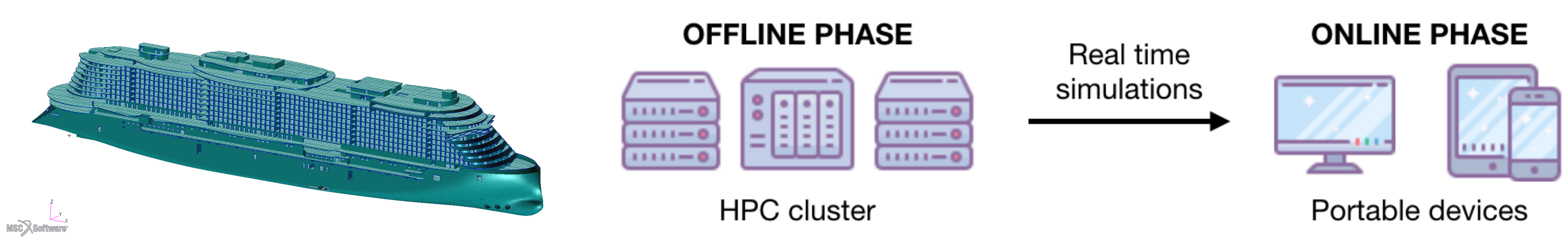
HEXAGON MSC Software



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,

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

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

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:

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

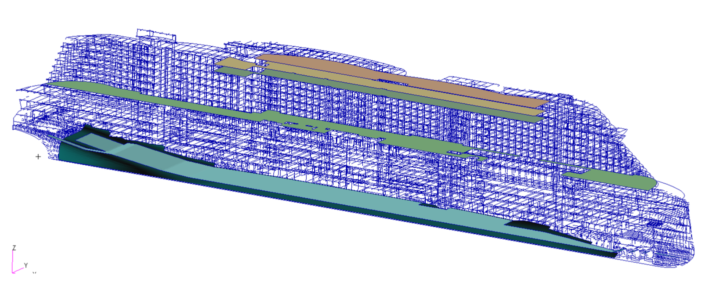
Athena

`github.com/mathLab/ATHENA`

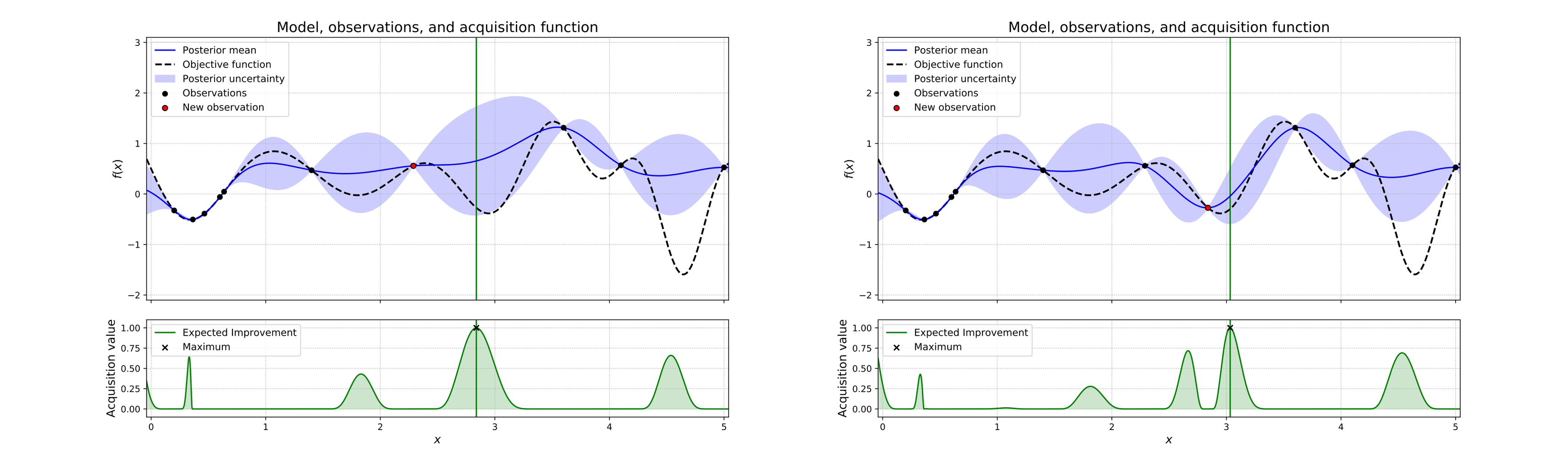
3 - Bayesian optimization

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

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

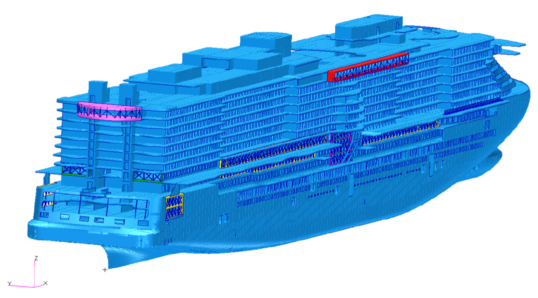


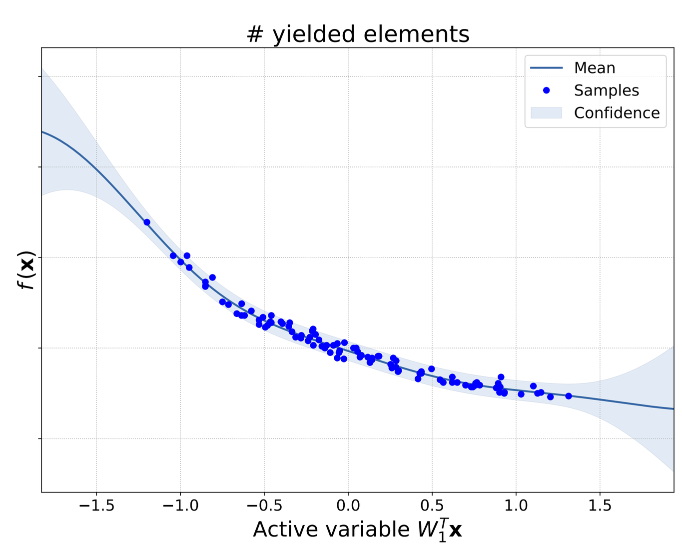
We maximize the **Expected Improvement** acquisition function, depicted in green below with an illustrative example, to select the next sample to evaluate. Our design inputs are the thickness of 6 regions of the hull.

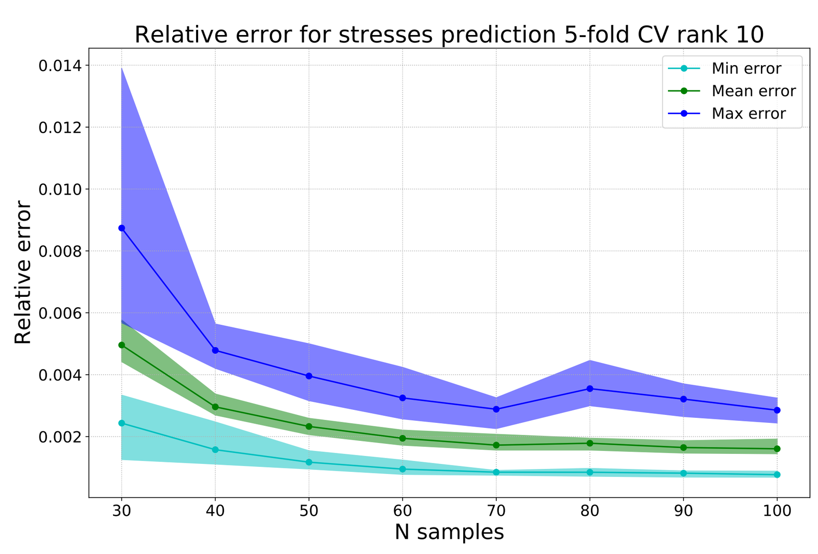


4 - Solution fields and constraints prediction

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.

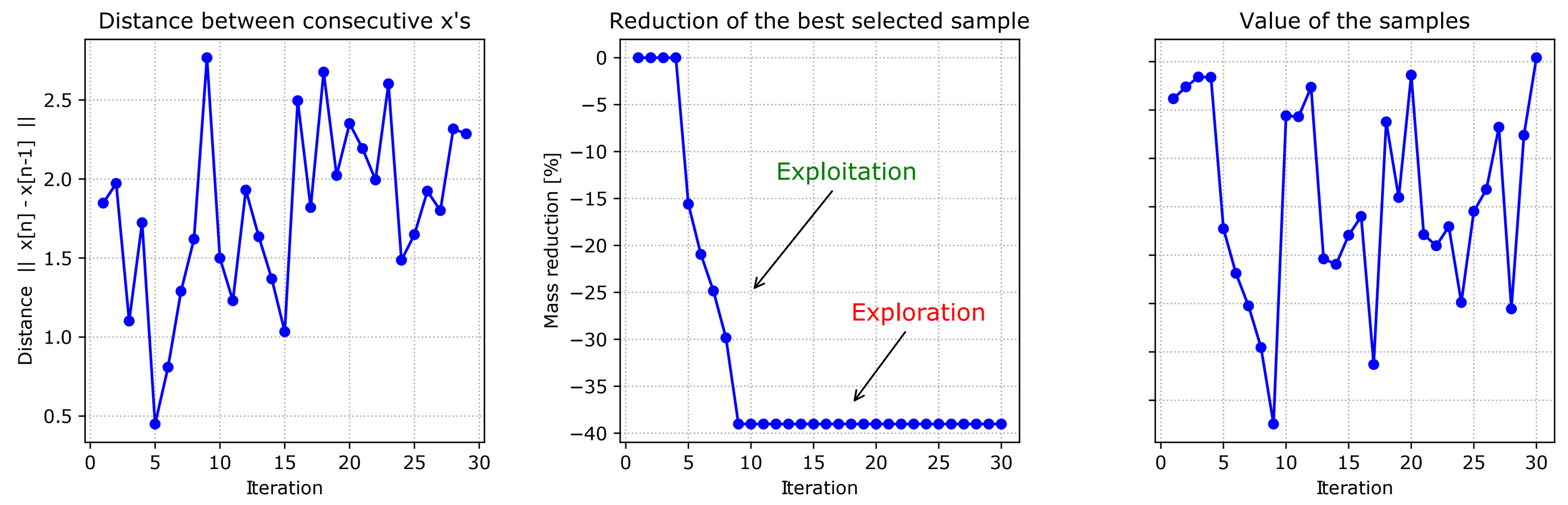






5 - Numerical results

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.

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