# Supporting Expensive Physical Models With Geometric Moment Invariants to Accelerate Sensitivity Analysis for Shape Optimisation

Shahroz Khan* and Panagiotis Kaklis †
*Department of Naval Architecture, Ocean and Marine Engineering, University of Strathclyde, Glasgow, United Kingdom.*

Andrea Serani ‡and Matteo Diez §
*CNR-INM, National Research Council-Institute of Marine Engineering, Rome, Italy*

**In this work, we proposed a computationally inexpensive Parametric Sensitivity Analysis (PSA) approach, which, to evaluate the parameters' sensitivity, substitutes design's physical quantities by the geometric ones, such as geometric moments and their invariants. Physical quantities rely strongly on design's geometry, and the evaluation of geometric properties is computationally inexpensive; therefore, our approach utilises these quantities to aid users in making informed decisions on parametric sensitivities. The feasibility of the proposed method is tested on a ship hull parameterised with 27 parameters. The sensitives of these 27 parameters are assessed with a global variance-based PSA first with respect to wave resistance coefficient ($c_w$), which is a crucial physical quantity for ship design, and then with respect to the second-order geometric moment invariants ($\mathrm{M}^2$). The parametric sensitives obtained with two quantities showed a good correlation, i.e., the four most sensitive parameters to $c_w$ are also sensitive to $\mathrm{M}^2$. Finally, two design spaces are constructed with only the sensitive parameters evaluated from the two quantities and shape optimisation is performed in both design spaces to optimise the hull shape for $c_w$. The $c_w$ values of optimised shapes obtained from the two spaces showed only $2.5589\%$ of difference. Moreover, the computational cost to perform PSA and shape optimisation with $c_w$ and $\mathrm{M}^2$ is approximately 375 and 9.5 hours, respectively. These results indicate that PSA performed with moments can reasonably estimate parameters' sensitivity to the design's physics with considerably reduced computational cost.**

## I. Introduction

With the advancements in computational power, Computer-Aided Design (CAD) and physics-based simulation tools have been a driving innovation in engineering and industrial product design. These technologies have outdated the costly and time-consuming physical prototyping and testing processes with effective shape optimisation pipelines integrated with digital twins. These pipelines are usually composed of three main components; CAD-based parametric techniques, optimisers and design's performance evaluation solvers such as Computational Fluid Dynamics (CFD) and Finite Elements Analysis (FEA). At first, design parameterisation creates a rich design space, which is later coupled with an optimiser and a solver to initiate shape optimisation [1]. Here, the optimiser first searches a parametric instance. The shape modification method then updates the initial design based on this instance, and the solver evaluates its performance to drive the exploration towards a global optimum.

The construction of parametric models, especially for freeform shapes, is an intricate process, and the decision on the number of parameters is critical. It is commonly made intuitively based on designers' or engineers' experience while considering a few essential factors: (1) all the critical features of the shape are parameterised [2], and (2) modification of the parameters does not create impractical or invalid geometries [3]. Even though designers try to favour parametrisation with many parameters for high design variation; however, in optimisation, this increases the risk of the

*Marie Skłodowska-Curie Research Fellow, Department of Naval Architecture, Ocean and Marine Engineering, University of Strathclyde, 16 Richmond St, Glasgow G1 1XQ, United Kingdom.
†Reader, Department of Naval Architecture, Ocean and Marine Engineering, University of Strathclyde, 16 Richmond St, Glasgow G1 1XQ, United Kingdom.
‡Research Scientist, CNR-INM Rome, Via di Vallerano 139, 00128.
§Senior Research Scientist, CNR-INM Rome, Via di Vallerano 139, 00128, AIAA Member.

curse of dimensionality resulting in high computational cost as it requires extensive exploration of high-dimensional design space for global optima and evaluation of a large number of designs with time expensive physical simulations [4].

Parametric sensitivity analyses (PSA) are widely used to support the robustness and efficiency in shape optimisation. It enables the designers to identify the subset of most sensitive parameters to the design's physics variability [5]. Once obtained, insensitive parameters can be excluded or fixed to reduce the dimensionality of the design space, thereby facilitating the efficient exploration of the design space. However, for complex engineering problems involving free shapes (e.g., ship hulls), PSA implementation often suffers from high computational cost, especially when the design's physics is computationally costly to evaluate [6, 7].

In this work, we aim to tackle these changelings in the context of computationally inexpensive PSA, which, instead of the design's physical properties, adopts geometric ones to access parametric sensitives. The physical properties rely strongly on design geometry, and the evaluation of geometric properties is comparatively computationally inexpensive [8, 9]. Therefore, we propose a geometry-based sensitivity analyses approach, which uses integral properties, such as geometric moments. The selection of geometric moments in our work for evaluating parametric sensitivities at the early design stage is made based on two fundamental insights; geometric moments of a shape:

1) are the intrinsic properties of its underlying geometry, which provides critical design cues to aid it's CAD [8], and
2) are the unifying medium between geometry and its physical evaluation [9].

From a geometric point of view, these moments can provide overall volume enclosed by the shape, its centre of mass, a moment of inertia and can evaluate the distribution of volume in different coordinate directions. More interestingly, these have been widely utilised to measure the extrinsic geometric similarity, which is used for object recognition [10], shape retrieval [11], rigid body transformation [12], etc. Moreover, shape integrals also provide a geometric foundation for many physical analyses of design, such as structural analysis [13], meshless physical analysis [9], governing equations of motion [14], fluid simulations [15, 16], hydrodynamic and hydrostatic stability [17], etc.

Therefore, we perform an experimental study to prove that geometric moments can ease the designer for efficient and appropriate design parameterisation and provide a preliminary estimation of parameters' sensitivity on design physics at the initial stage. We first performed a global variance-based sensitivity analysis [5] concerning wave resistance coefficient ($c_w$) and a set of second-order volume moments invariant to translation and scaling [18]. Here, the former is a physical quantity and computationally expensive to evaluate, and the latter is purely a geometric one. Afterwards, we perform a correlation study to identify a common set of sensitive parameters between two quantities. Two different Gaussian process-based surrogate models are developed with a set of sensitive parameters obtained with moments and $c_w$, which were then connected with an optimiser to obtain optimal designs.

## II. Proposed Approach

This section gives general assumptions set for the proposed approach along with a brief overview of sensitivity analysis and the mathematical formulation of geometric moments and their invariants.

Let a parametric design, $\gamma$, is represented with a set of $n$ continuous design parameters $\mathbf{X} = \{X_k, k = 1, 2, \dots, n\} \in \mathcal{X} \subseteq \mathbb{R}^n$, whose certain realisation is represented as $\mathbf{x} = \{x_k, k = 1, ..., n\}$. Here $\mathcal{X}$ is the $n$-dimensional solution/design space, which is bounded with lower $\mathbf{x_m^l}$ and upper $\mathbf{x_m^u}$ limits of parameters (i.e., $\mathcal{X} := \{x_k^l \leq x_k \leq x_k^u, \forall k \in \{1, 2, \dots n\}\}$). Moreover, all the elements of $\mathbf{X}$ are also assumed to be statistically independent from each other, i.e., $p_{\mathbf{x}}(\mathbf{x}) = \prod_{k=1}^{n} p_{X_k}(x_k)$, where $p_{\mathbf{X}}(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$ represents the Probability Density Function (PDF) of $\mathbf{X}$ and $p_{X_k}(x_k)$ is the marginal PDF of $X_k$. Now, the objective is to access the sensitivity indices, $\{\mathcal{I}_1, \mathcal{I}_2, \dots, \mathcal{I}_n\}$, of each element of $\mathbf{X}$ with respect to a quantity of interest (QoI), which is evaluated using a square-integrable vector function $g : \mathcal{X} \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$. Afterwards, we find a set of $m$ sensitive or significant parameters whose sensitivity index is greater than a significant threshold, $\epsilon$, where $m$ is favourable to be less than $n$.

### A. Sensitivity analysis

In a parametric study, sensitivity analysis enables identifying the local or global influence of a single or set of parameters on the QoI, respectively. In other words, it provides insight into the variability of QoI, which in our case are the geometric moments contributed by input parameters. In a local sensitivity analysis, the change in QoI is evaluated with respect to variation in a single parameter. In the global sensitivity analysis, variability in QoI is measured against the variation in all parameters over the entire design space. This allows users to evaluate the relative contribution of each parameter to QoI's output variation. In literature, different types of local and global sensitivity analyses, such as variance-based (or Sobol's method), derivative-based, density-based sensitivity, elementary effects test (or Morris method) [19], etc., have been proposed.

Among these techniques, global variance-based methods like Sobol's analysis is suitable for complex nonlinear and non-additive models; therefore, is well received in different design applications and thus used in the current study. This method investigates how much of the overall variance of QoI is achieved due to the variability of a single or collection of design parameters. This variance is usually measured with *First-order indices* (or *main effects*) or *total-order indices* (or *total effects*). The former quantifies the direct contribution to QoI variance from an individual parameter. The latter approximates the overall contribution from a parameter considering its direct effect and interactions with all the other design parameters.

### B. Geometry-Based Sensitivity Analysis

In our approach, QoIs are the integral characteristics, such as geometric moments of various orders. As mentioned earlier, in physical analyses, such as Finite Element Method (FEM) and Computational Fluid Dynamics (CFD), these moments are used for displacement, deflection, shear stress, stability [17], governing equation of motions [14] and incompressible flows [15, 16], etc. Recently, meshfree methods have also been developed in FEA [9], which uses moment-based representations of shape to aid the interoperability between CAD representation and its physics. Moreover, for floating structures such as ships, moments also play a critical role in determining their initial stability in the water. These applications motivate us to create a direct relation for the parameter sensitive to the moment and study if this makes a similar sensitivity effect on its associated physics. Moreover, performing computationally effective sensitivity analysis at the preliminary stage can also provide a reasonable estimation of the sensitivity of parameters, thereby expediting the entire product development process.

#### *1. Geometric Moments and Invariants*

Consider $\gamma$ as an arbitrary shape in a three-dimensional (3D) Euclidean space. The geometric measure of $\gamma$ in term of moments can be defined as Riemann integrals and represented as:

$$M^{p,q,r}(\gamma) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} x^p\ y^q\ z^r\ \rho(x, y, z)\ \mathrm{d}x\mathrm{d}y\mathrm{d}z, \quad p, q, r \in \{0, 1, 2, \dots\}. \tag{1}$$

Eq. 1 give a $s^{th}$ order geometric moment for $\gamma$ of 3D density function $\rho(x, y, z)$, where $s = q + p + r$. If $\rho(x, y, z)$ is piecewise continuous and bounded in 3D Euclidean space then moments for $\gamma$ of any order can be evaluated. With Eq. 1 can construct a moment-vector, $\mathbf{M}^s$, containing all the moments up to $s^{th}$ order to represent a shape as

$$\mathbf{M}^s = \left[ M^{p,q,r}(\gamma), \forall p, q, r \in \{0, 1, 2, \dots, s\} \mid p + q + r \leq s \right]. \tag{2}$$

The zeroth and first order moments, $M^{0,0,0}(\gamma)$, $M^{1,0,0}(\gamma)$, $M^{0,1,0}(\gamma)$, and $M^{0,0,1}(\gamma)$, are most widely used and correspond to the object volume, $V = M^{0,0,0}(\gamma)$ and the coordinates of the center-of-mass ($\mathbf{c}(\gamma)$):

$$\mathbf{c}(\gamma) = \begin{bmatrix} c_x \\ c_y \\ c_z \end{bmatrix} = \begin{bmatrix} \frac{M^{1,0,0}(\gamma)}{M^{0,0,0}(\gamma)} \\ \frac{M^{0,1,0}(\gamma)}{M^{0,0,0}(\gamma)} \\ \frac{M^{0,0,1}(\gamma)}{M^{0,0,0}(\gamma)} \end{bmatrix} \tag{3}$$

Moreover, the moments of second order can be organised in a second rank tensor, the moment of inertia tensor (MoI), which is represented as follows:

$$\mathrm{MoI} = \begin{bmatrix} M^{0,2,0}(\gamma) + M^{0,0,2}(\gamma) & -M^{1,1,0}(\gamma) & -M^{1,0,1}(\gamma) \\ -M^{1,1,0}(\gamma) & M^{2,0,0}(\gamma) + M^{0,0,2}(\gamma) & -M^{0,1,1}(\gamma) \\ -M^{1,0,1}(\gamma) & -M^{0,1,1}(\gamma) & M^{2,0,0}(\gamma) + M^{0,2,0}(\gamma) \end{bmatrix} \tag{4}$$

The moments in $\mathbf{M}^s$ are variant to rigid and non-rigid transformations, such as translation, rotation and scaling [18]. However, most of the physical quantities are invariant to either all or some of these transformations. For instance, evaluating $c_w$ for the ship is invariant to translation and scaling if assessed at a certain Froude number. Therefore, to measure the sensitives of the parameters with respect to the geometry, the invariants of these moments with respect to translation and scaling have to be evaluated.

If the Eq. (1) is evaluated while placing $\gamma$ at its cenertiod, $\mathbf{c}(\gamma)$ then it provides a central moment of $s^{th}$ order, which is invariant to the translation and is expressed as:

$$\mu^{p,q,r}(\gamma) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} (x - c_x)^p \ (y - c_y)^q \ (z - c_z)^r \ \rho(x, y, z) \ \mathrm{d}x\mathrm{d}y\mathrm{d}z. \tag{5}$$

It is note worthy that as $\gamma$ is place at the $\mathbf{c}(\gamma)$; therefore the central moment of first order is zero, i.e., $[\mu^{1,0,0}, \mu^{0,1,0}, \mu^{0,0,1}] = 0$. Assume that the object is scaled by factor $\lambda$ then

$$\hat{\mu}^{p,q,r}(\gamma) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} (x - c_x)^p \ (y - c_y)^q \ (z - c_z)^r \ \rho(\frac{x}{\lambda}, \frac{y}{\lambda}, \frac{z}{\lambda}) \ \mathrm{d}x\mathrm{d}y\mathrm{d}z, \tag{6}$$

$$= \lambda^{p+q+r+3}\mu^{p,q,r}(\gamma). \tag{7}$$

So,

$$\zeta^{p,q,r} = \frac{\mu^{p,q,r}}{(\mu^{0,0,0})^{1+(p+q+r)/3}} \tag{8}$$

is an invariant moment form for $\gamma$ under uniform scaling and translation.

*2. Sensitivity index with respect to moments*

Unlike physics, which are mostly scale quantities, the moment of any order is a vector quantity composed of multiple term with different order of each of the $p$-, $q$- and $r$-th component. For instance, there are six different moments of second order:

$$[\zeta^{2,0,0}(\gamma), \zeta^{0,2,0}(\gamma), \zeta^{0,0,2}(\gamma), \zeta^{1,1,0}(\gamma), \zeta^{1,0,1}(\gamma), \zeta^{0,1,1}(\gamma)]. \tag{9}$$

All the terms in moment-vector $\mathbf{M}^s$ represents $\gamma$ up to $s^{th}$ order. Therefore, we first construct a sensitivity matrix, shown in Eq. (10), which contains the sensitivity indices of all parameters in $\mathbf{X}$ with respect to all terms of $\mathbf{M}^s$.

$$\mathbf{I}^s = \begin{bmatrix} I_1^{0,0,0} & I_1^{1,0,0} & \dots & I_1^{p,0,0} & I_1^{p,1,0} & \dots & I_1^{p,q,0} & I_1^{p,q,1} & \dots & I_1^{p,q,r} \\ I_2^{0,0,0} & I_2^{1,0,0} & \dots & I_2^{p,0,0} & I_2^{p,1,0} & \dots & I_2^{p,q,0} & I_2^{p,q,1} & \dots & I_2^{p,q,r} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ I_n^{0,0,0} & I_n^{1,0,0} & \dots & I_n^{p,0,0} & I_n^{p,1,0} & \dots & I_n^{p,q,0} & I_n^{p,q,1} & \dots & I_n^{p,q,r} \end{bmatrix} \tag{10}$$

All moments in $\mathbf{M}^s$ has the same nature when it comes to representing geometry. Therefore, the overall sensitivity index, $\mathcal{I}_k^s$, of an $k^{th}$ parameter is evaluated by summing its sensitivity indices with respect to all the moments in $\mathbf{M}^s$ as

$$\mathcal{I}_k^s = \sum_{p=0}^{s}\sum_{q=0}^{s}\sum_{r=0}^{s} w_k^{p,q,r}, \quad \forall k \in \{1, 2, \dots, n\}, \tag{11}$$

where

$$w_k^{p,q,r} = \begin{cases} I_k^{p,q,r} & \text{if} \quad p + q + r \le s \\ 0 & \text{otherwise} \end{cases}. \tag{12}$$

To ease the visual analysis of the sensitivity indices they are normalised to have a unit norm as:

$$\mathcal{I}_k^s \mapsto \frac{\mathcal{I}_k^s}{\sum_{k=1}^{n} \mathcal{I}_k^s}. \tag{13}$$

Eq. 13 give sensitivity bounded between 0 and 1.0. Parameters having an index value close to 1.0 have more impact on the variability of QoI's. After obtaining the sensitivity indices, the total $n$ parameters are divided into two subsets containing $m$ significant and $n - m$ insignificant parameters. The significant parameters have a sensitivity index greater or equal to the significant threshold, $\epsilon$. For complex analyses, $\epsilon = 0.05$ is widely used [20].

*3. Optimisation*

Once a set of $m$ significant parameters are identified, they are first used to construct an $m$-dimensional sensitivities space, $\mathcal{X}_M \subseteq \mathbb{R}^m$, which is then re-sampled to build a dataset along with the design's functional QoI. This dataset is used to construct a surrogate model, which is then connected with an optimiser to explore the significant design space, coupled with the surrogate model, for an optimal design.

## III. Test Case

The proposed method is demonstrated for the hull-form optimisation of the DTMB 5415 model (see Fig. 1), an early and open to the public version of the USS Arleigh Burke destroyer DDG 51, extensively used as an international benchmark for shape optimisation problems [21, 22]. Table 1 summarises the main characteristics of the hull and test conditions.

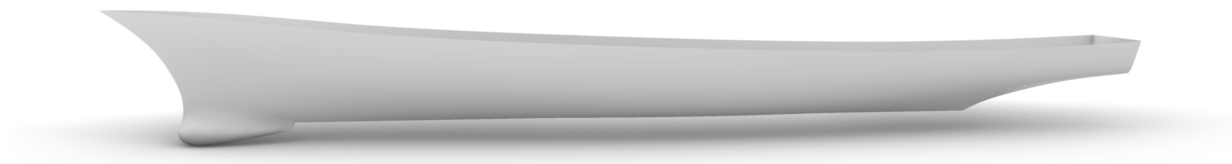

**Fig. 1 CAD geometry of DTMB 5415 naval ship model used as test case for the proposed approach.**

**Table 1 DTMB 5415 original (model scale) hull main particulars.**

| Quantity | Symbol | Unit | Value |
|---|---|---|---|
| Displacement | $\nabla$ | $m^3$ | 0.549 |
| Length between perpendiculars | $L_{\mathrm{pp}}$ | m | 5.720 |
| Beam | $B$ | m | 0.760 |
| Draft | $T$ | m | 0.248 |
| Longitudinal center of gravity | LCG | m | 2.884 |
| Vertical center of gravity | VCG | m | 0.056 |
| Water density | $\rho$ | $kg/m^3$ | 998.5 |
| Kinematic viscosity | $\nu$ | $m^2/s$ | 1.09E-6 |
| Gravity acceleration | $g$ | $m/s^2$ | 9.803 |
| Froude number | Fr | – | 0.250 |

The optimisation aims to reduce the (model-scale) calm-water wave resistance coefficient ($c_w$) at Froude number equal to 0.25.

### A. Shape Modification Method

The shape modification is defined using a recursive combination of $n = 27$ shape modification vectors over a hyper-rectangle embedding the demi hull:

$$\boldsymbol{\psi}_i(\boldsymbol{\zeta}) \;:\; \mathcal{A} = [0, L_{\zeta_1}] \times [0, L_{\zeta_2}] \times [0, L_{\zeta_3}] \in \mathbb{R}^3 \longrightarrow \mathbb{R}^3, \tag{14}$$

with $i = 1, \ldots, n$. Specifically,

$$\boldsymbol{\delta}(\boldsymbol{\zeta}, \mathbf{x}) = \boldsymbol{\delta}_M, \tag{15}$$

where

$$\boldsymbol{\delta}_i(\boldsymbol{\zeta}, \mathbf{x}) = x_i \boldsymbol{\psi}_i(\boldsymbol{\zeta}), \quad \text{with} \quad \begin{cases} \boldsymbol{\zeta} = \boldsymbol{\zeta} + \boldsymbol{\delta}_{i-1} \\ \boldsymbol{\delta}_1 = 0 \end{cases} \tag{16}$$

The coefficients $\{x_i, i = 1, \ldots, n \in \mathbb{R}\}$ are the design parameters and forms a 27−dimensional initial (original) design space $\mathcal{X}$. For modification the shape functions are defined as:

$$\boldsymbol{\psi}_i(\boldsymbol{\zeta}) := \prod_{j=1}^{3} \sin\left(\frac{a_{ij}\pi\zeta_j}{L_{\zeta_j}} + r_{ij}\right) \mathbf{e}_{q(i)}. \tag{17}$$

In Eq. (17), $\{a_{ij}, j = 1, 2, 3\} \in \mathbb{R}$ define the order of the function along $j$-th axis; $\{r_{ij}, j = 1, 2, 3\} \in \mathbb{R}$ are the corresponding spatial phases; $\{L_{\zeta_j}, j = 1, 2, 3\} \in \mathbb{R}$ are the hyper-rectangle edge lengths; $\mathbf{e}_{q(i)}$ is a unit vector. Modifications are applied along $\zeta_1$, $\zeta_2$, or $\zeta_3$, with $q(i) = 1, 2,$ or $3$ respectively. Details of setting parameters can be found in [23].

## IV. Results and Discussion

In this section, we first discuss the sensitivity analysis results performed with respect to $\mathbf{M}^2$ and $c_w$ along with the correlation between the results. Afterwards, we present the results of the surrogate modelling and the optimisation performed in the sensitivity spaces evaluated with $\mathbf{M}^2$ and $c_w$.

### A. Sensitivity Analysis

First, a 27-dimensional design space is created with original $n = 27$ design parameters to commence the sensitivity analysis, which was sampled using Monte-Carlo sampling with $S = 9000$ samples. Afterwards, second-order moment invariants ($\mathbf{M}^2$) and wave-resistance coefficient ($c_w$) of design were evaluated, and two different datasets were created, first containing the design parameter values as the dependent variable and $c_w$ as independent variables. $c_w$ values are obtained using the code WARP (Wave Resistance Program), developed at CNR-INSEAN. Wave resistance computations are based on linear potential flow theory using Dawson (double-model) linearisation [24]. The second dataset is composed of design parameters and $\mathbf{M}^2$ as independent variables. Sobol's global sensitivity analysis is performed using both datasets, whose results are shown in Figure 2.

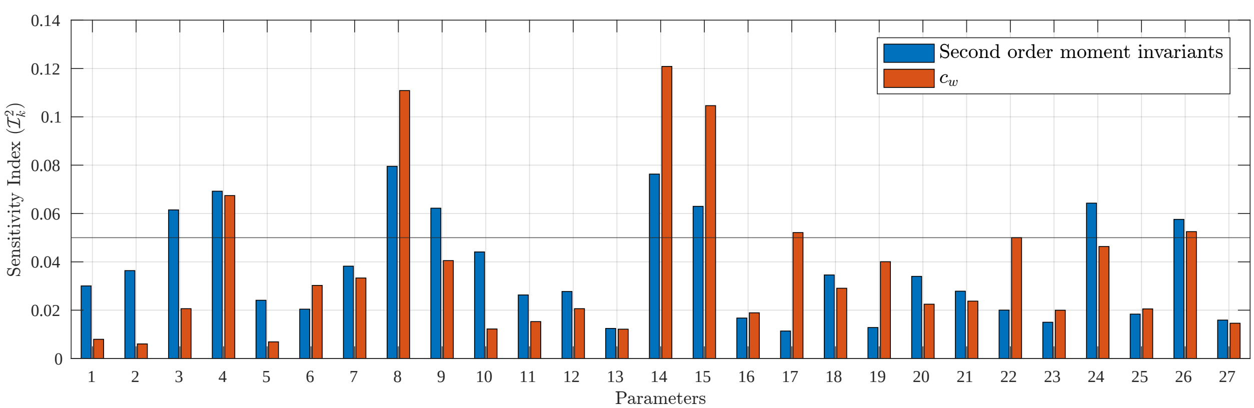


**Fig. 2 Sensitivity indices all 27 design parameters obtained using Eq. (13) with respect to $c_w$ and second order moment invariants.**

To select the set of $m$ sensitive parameters the significant threshold set to $\epsilon = 0.05$. It can be seen that in case of $c_w$, seven out of 27 parameters, $X_4$, $X_8$, $X_{14}$, $X_{15}$, $X_{17}$, $X_{22}$ and $X_{26}$ has the sensitivity index greater than $\epsilon$ and thus regarded as the most sensitive parameters with respect to $c_w$. Among these parameters, $X_{14}$, $X_8$ and $X_{15}$ have substantially high sensitivity index and $X_{17}$, $X_{22}$ and $X_{26}$ have the sensitivity index close to $\epsilon$. In case of $\mathbf{M}^2$, also in total seven parameters, $X_3$, $X_4$, $X_8$, $X_{14}$, $X_{15}$, $X_{24}$ and $X_{26}$, have sensitivity index higher than $\epsilon$. It is interesting to note that out of these seven sensitive parameters, five of them, $X_4$, $X_8$, $X_{14}$, $X_{15}$ and $X_{26}$, are also sensitive in case of $c_w$. More importantly, the parameters, $X_4$, $X_{14}$, $X_8$ and $X_{15}$, are the top four sensitive parameters with respect to both $c_w$ and moments. Using the top seven parameters sensitive to $c_w$ and $\mathbf{M}^2$, two different seven-dimensional design spaces, $\mathcal{X}_{c_w}$ and $\mathcal{X}_M$, are created, respectively.

**Table 2 Error values obtained during the training of surrogate models $g_{c_w}$ and $g_M$.**

| Surrogate models | $g_{c_w}$ | $g_M$ |
|---|---|---|
| Dimensions | 7 | 7 |
| Cross-validation-MSE | 0.2683 | 0.2716 |
| $R^2$ | 0.9595 | 0.9576 |

### B. Surrogate Modelling and Optimisation

To initiate optimisation, we first construct two surrogate models, $g_{c_w}$ and $g_M$ one in a design space constructed with the set significant parameters identified with $c_w$ ($\mathcal{X}_{c_w}$) and other with parameters identified significant for $\mathbf{M}^2$ ($\mathcal{X}_M$). For constructing the surrogate model, we utilised Gaussian process regression (GPR), which is a non-parametric Bayesian approach [25], which have been used in different design applications [26]. It maps the nonlinear and globally coupled relationship between inputs and outputs sampled from a theoretically infinite-dimensional normal distribution and any finite number of samples in the input space, which follow a corresponding joint (multivariate) Gaussian distribution. The main advantages of GPR over other modelling techniques are, it can: (1) map relationship between inputs and outputs with small data size and, (2) easily handle noise in the data, thus, avoid over-fitting, and (3) optimise hyper-parameters from training data to increase the fit accuracy. The $R^2$ and cross-validation mean squared error (MSE) values for both models are shown in the Table 2.

Afterwards, two different optimisation experiments are performed to optimise the parent hull in order to reduce $c_w$. First, the optimisation is performed in $\mathcal{X}_{c_w}$ and design were during this optimisation are evaluated with the surrogate model $g_{c_w}$. The second optimisation is carried out in $\mathcal{X}_M$, and during the exploration of this space, designs were evaluated with the surrogate model $g_M$. For optimisation, we utilised the Jaya Algorithm (JA) [27], which is a simple yet effective meta-heuristic optimisation technique whose performance has been proven in various engineering applications. As JA is a stochastic meta-heuristic technique, which may provide different results in each run, 100 different optimisation runs were performed. In each run, a total of 1500 iterations were conducted. Figure 3 shows the average, maximum and minimum values of $c_w$ during 100 runs performed in both design spaces.

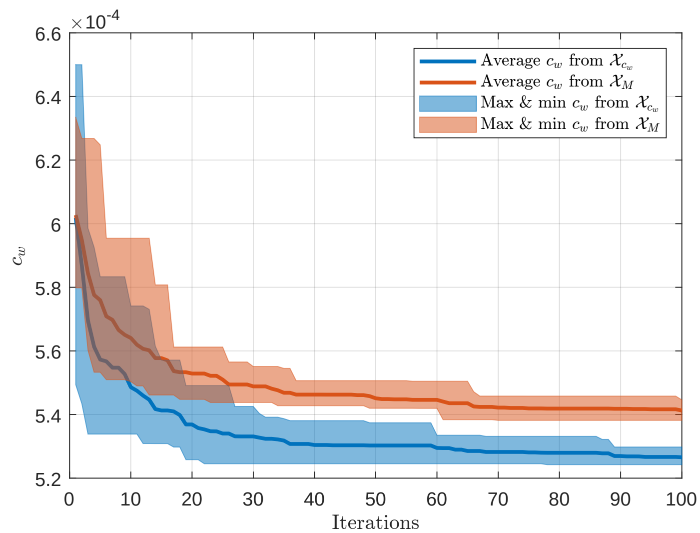


**Fig. 3 Plots showing the average, aximum and minimum values of $c_w$ versus number of optimisation iterations performed in $X_{c_w}$ and $X_M$ over 100 optimisation runs.**

Figure 4 show the designs generated form $\mathcal{X}_{c_w}$ and $\mathcal{X}_M$ at the end of the optimisation, whose $c_w$ values are 5.2241E-4 and 5.3578E-4, respectively. It is interesting to note that both designs have similar shapes, especially for the part below the waterline. Their $c_w$ values are also close to each other, with a difference of only 2.5589% in terms of absolute percentage error.

The computational cost to perform sensitivity analysis with respect to $c_w$ and $\mathbf{M}^2$ and to perform optimisation in $\mathcal{X}_{c_w}$ and $\mathcal{X}_M$ is approximately 375 and 9.5 hours, respectively. This shows that performing sensitivity analysis with

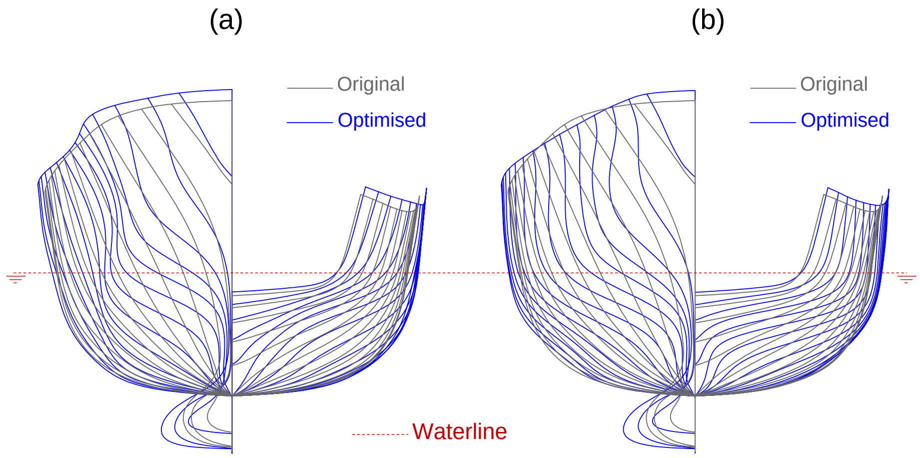


**Fig. 4 Comparison between the baseline design and optimised designs obtained from the lower-dimensional design spaces, $\mathcal{X}_{c_w}$ and $\mathcal{X}_M$.**

geometric moments can estimate the parameters' sensitivity concerning physics, at least in hydrodynamic analysis, with extensively reduced computational cost.

## V. Conclusion & Final Paper Contents

This work describes our quest to support computationally demanding physical models with computationally efficient geometric quantities such as geometric moments and their invariants. Using these geometric quantities, we proposed a method to expedite the parametric sensitivity analysis in the context of shape optimisation of 3D free-form shapes such as ship hulls. The selection of geometric properties is motivated by the fact that the moments of solid shapes are intrinsic properties of their underlying shape that can provide essential design indications to facilitate designers in Computer-aided Design. Computing moments is also vital for physics-based simulations that help in improving realism in animations. To prove if geometric moments can benefit designers as a prior check on the sensitivity of parameters, we performed two different PSA; first with wave-resistance coefficient ($c_w$), which is a physical property and then with second-order geometric moment invariants ($\mathbf{M}^2$). The results showed a good correlation between the sensitive parameters obtained from both experiments. Afterwards, two different design spaces were constructed, one with sensitive parameters obtained with $c_w$ and the other with moments. Shape optimisation is performed in both spaces in connection with the surrogate models. Final optimisation results showed that the design generated from both spaces has similar features, and $c_w$ values are close with only 2.5589% of difference.

As future work, we would like to study the effect of higher-order geometric moments on the sensitivity of parameters, specifically third-order geometric moment invariants ($\mathbf{M}^3$) as similar to $c_w$ it is primarily affected by the variation in shape along its longitudinal direction.

## Acknowledgements

This work's first and second authors have received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 860843. The third and fourth authors are grateful to the US Office of Naval Research for its support through NICOP grant N62909-18-1-2033.

## References

[1] Khan, S., Serani, A., Diez, M., and Kaklis, P., "Physics-informed feature-to-feature learning for design-space dimensionality reduction in shape optimisation," *AIAA Scitech 2021 Forum*, 2021, p. 1235.

[2] Khan, S., Gunpinar, E., and Dogan, K. M., "A novel design framework for generation and parametric modification of yacht hull surfaces," *Ocean Engineering*, Vol. 136, 2017, pp. 243–259.

[3] Khan, S., and Awan, M. J., "A generative design technique for exploring shape variations," *Advanced Engineering Informatics*, Vol. 38, 2018, pp. 712–724.

[4] Chen, W., Fuge, M., and Chazan, J., "Design manifolds capture the intrinsic complexity and dimension of design spaces," *Journal of Mechanical Design*, Vol. 139, No. 5, 2017.

[5] Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., and Tarantola, S., *Global sensitivity analysis: The primer*, John Wiley & Sons, 2008.

[6] Sheikholeslami, R., Razavi, S., Gupta, H. V., Becker, W., and Haghnegahdar, A., "Global sensitivity analysis for high-dimensional problems: How to objectively group factors and measure robustness and convergence while reducing computational cost," *Environmental modelling & software*, Vol. 111, 2019, pp. 282–299.

[7] Khan, S., and Kaklis, P., "From regional sensitivity to intra-sensitivity for parametric analysis of free-form shapes: Application to ship design," *Advanced Engineering Informatics*, Vol. 49, 2021, p. 101314.

[8] Krishnamurthy, A., and McMains, S., "Accurate GPU-accelerated surface integrals for moment computation," *Computer-Aided Design*, Vol. 43, No. 10, 2011, pp. 1284–1295.

[9] Taber, A., Kumar, G., Freytag, M., and Shapiro, V., "A moment-vector approach to interoperable analysis," *Computer-Aided Design*, Vol. 102, 2018, pp. 139–147.

[10] Atrevi, D. F., Vivet, D., Duculty, F., and Emile, B., "A very simple framework for 3D human poses estimation using a single 2D image: Comparison of geometric moments descriptors," *Pattern Recognition*, Vol. 71, 2017, pp. 389–401.

[11] Luciano, L., and Hamza, A. B., "A global geometric framework for 3D shape retrieval using deep learning," *Computers & Graphics*, Vol. 79, 2019, pp. 14–23.

[12] Bronstein, A. M., Bronstein, M. M., and Kimmel, R., *Numerical geometry of non-rigid shapes*, Springer Science & Business Media, 2008.

[13] Kim, B. W., Hong, S. Y., Kyoung, J. H., and Cho, S. K., "Evaluation of bending moments and shear forces at unit connections of very large floating structures using hydroelastic and rigid body analyses," *Ocean engineering*, Vol. 34, No. 11-12, 2007, pp. 1668–1679.

[14] Newman, J. N., *Marine hydrodynamics*, MIT press, 2018.

[15] Jin, P., Xie, B., and Xiao, F., "Multi-moment finite volume method for incompressible flows on unstructured moving grids and its application to fluid-rigid body interactions," *Computers & Structures*, Vol. 221, 2019, pp. 91–110.

[16] Fox, R. O., Laurent, F., and Vié, A., "Conditional hyperbolic quadrature method of moments for kinetic equations," *Journal of Computational Physics*, Vol. 365, 2018, pp. 269–293.

[17] Biran, A., and Pulido, R. L., *Ship hydrostatics and stability*, Butterworth-Heinemann, 2013.

[18] Xu, D., and Li, H., "Geometric moment invariants," *Pattern recognition*, Vol. 41, No. 1, 2008, pp. 240–249.

[19] Constantine, P. G., and Diaz, P., "Global sensitivity metrics from active subspaces," *Reliability Engineering & System Safety*, Vol. 162, 2017, pp. 1–13.

[20] Zhang, X.-Y., Trame, M. N., Lesko, L. J., and Schmidt, S., "Sobol sensitivity analysis: a tool to guide the development and evaluation of systems pharmacology models," *CPT: pharmacometrics & systems pharmacology*, Vol. 4, No. 2, 2015, pp. 69–79.

[21] Grigoropoulos, G., Campana, E., Diez, M., Serani, A., Goren, O., Sarioz, K., Danisman, D., Visonneau, M., Queutey, P., Abdel-Maksoud, M., et al., "Mission-based hull-form and propeller optimization of a transom stern destroyer for best performance in the sea environment," *Proceedings of the VII International Congress on Computational Methods in Marine Engineering-MARINE*, 2017.

[22] Serani, A., Diez, M., Wackers, J., Visonneau, M., and Stern, F., "Stochastic Shape Optimization via Design-Space Augmented Dimensionality Reduction and RANS Computations," *57th AIAA Aerospace Sciences Meeting, SciTech 2019*, Manchester Grand Hyatt San Diego, San Diego, California, January 7-11, 2019.

[23] Serani, A., D'Agostino, D., Campana, E. F., and Diez, M., "Assessing the Interplay of Shape and Physical Parameters by Unsupervised Nonlinear Dimensionality Reduction Methods," *Journal of Ship Research*, 2019.

[24] Dawson, C. W., "A practical computer method for solving ship-wave problems," *Proceedings of the 2nd International Conference on Numerical Ship Hydrodynamics*, Berkeley, 1977, pp. 30–38.

[25] Williams, C. K., and Rasmussen, C. E., *Gaussian processes for machine learning*, Vol. 2, MIT press Cambridge, MA, 2006.

[26] Masood, Z., Khan, S., and Qian, L., "Machine learning-based surrogate model for accelerating simulation-driven optimisation of hydropower Kaplan turbine," *Renewable Energy*, Vol. 173, 2021, pp. 827–848.

[27] Rao, R., "Jaya: A simple and new optimization algorithm for solving constrained and unconstrained optimization problems," *International Journal of Industrial Engineering Computations*, Vol. 7, No. 1, 2016, pp. 19–34.