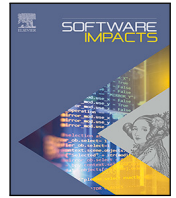


Contents lists available at [ScienceDirect](https://www.sciencedirect.com)

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Original software publication

PyGeM: Python Geometrical Morphing

Marco Tezzele ^{*}, Nicola Demo, Andrea Mola, Gianluigi Rozza*Mathematics Area, mathLab, SISSA, International School of Advanced Studies, Trieste, Italy*

ARTICLE INFO

Keywords:

Free form deformation
 Radial basis functions interpolation
 Inverse distance weighting
 Geometrical morphing
 Python

ABSTRACT

PyGeM is an open source Python package which allows to easily parametrize and deform 3D object described by CAD files or 3D meshes. It implements several morphing techniques such as free form deformation, radial basis function interpolation, and inverse distance weighting. Due to its versatility in dealing with different file formats it is particularly suited for researchers and practitioners both in academia and in industry interested in computational engineering simulations and optimization studies.

Code metadata

Current code version	2.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2020-59
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/9903556/tree/v1
Legal Code License	MIT License (MIT)
Code versioning system used	git
Software code languages, tools, and services used	Python
Compilation requirements, operating environments & dependencies	PyGeM requires <code>numpy</code> , <code>scipy</code> , <code>matplotlib</code> , <code>sphinx</code> (for the documentation) and <code>nose</code> (for local test). To enable the CAD submodule, the module <code>pythonocc-core</code> is required to deal with IGES files.
If available Link to developer documentation/manual	http://mathlab.github.io/PyGeM/
Support email for questions	marco.tezzele@sissa.it nicola.demo@sissa.it andrea.mola@sissa.it

Software metadata

Current software version	2.0
Permanent link to executables of this version	https://github.com/mathLab/PyGeM/releases/tag/v2.0
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/9903556/tree/v1
Legal Software License	MIT License (MIT)
Computing platforms/Operating Systems	Linux, OS X, Unix-like
Installation requirements & dependencies	PyGeM requires <code>numpy</code> , <code>scipy</code> , <code>matplotlib</code> , <code>sphinx</code> (for the documentation) and <code>nose</code> (for local test). To enable the CAD submodule, the module <code>pythonocc-core</code> is required to deal with IGES files.
If available, link to user manual - if formally published include a reference to the publication in the reference list	http://mathlab.github.io/PyGeM
Support email for questions	marco.tezzele@sissa.it nicola.demo@sissa.it andrea.mola@sissa.it

The code (and data) in this article has been certified as Reproducible by Code Ocean: (<https://codeocean.com/>). More information on the Reproducibility Badge Initiative is available at <https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals>.

^{*} Corresponding author.

E-mail addresses: marco.tezzele@sissa.it (M. Tezzele), nicola.demo@sissa.it (N. Demo), andrea.mola@sissa.it (A. Mola), gianluigi.rozza@sissa.it (G. Rozza).

<https://doi.org/10.1016/j.simpa.2020.100047>

Received 25 November 2020; Accepted 30 November 2020

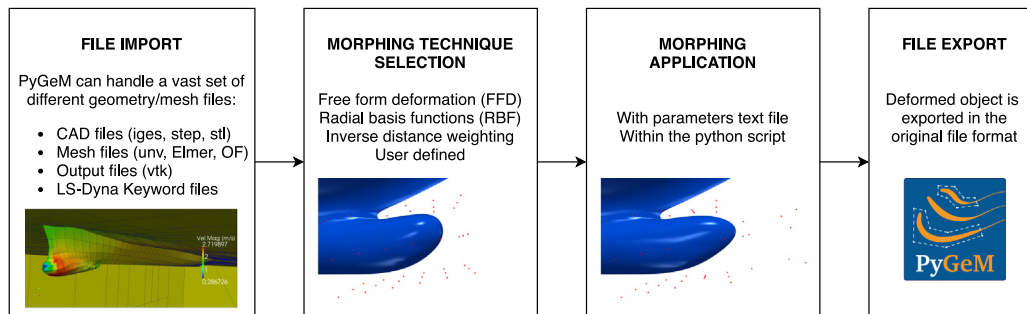


Fig. 1. PyGeM complete usage workflow. The coordinates of the points to morph can be read from different file formats. After selecting the proper parametrization technique and the corresponding parameters, we can export the deformed geometry into the original file format.

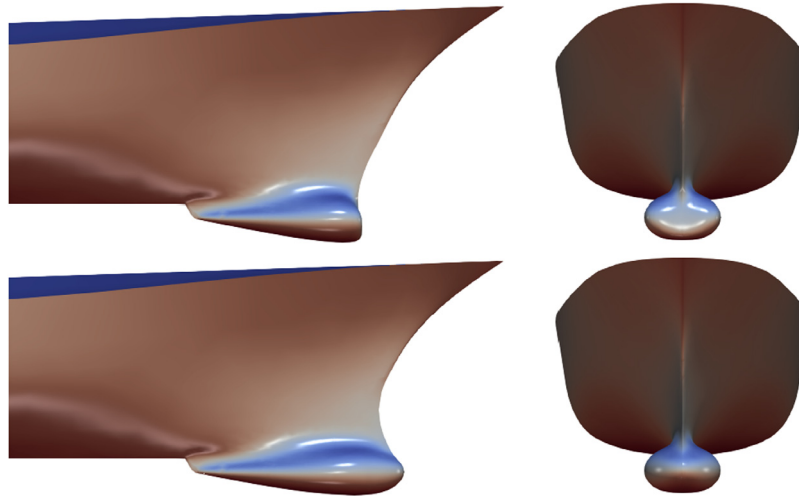


Fig. 2. Examples of two deformation on a naval hull, from lateral and frontal views.

1. The PyGeM package

In many simulation based processes, the performances of a certain product have to be evaluated varying the shape of the object itself. In all these parametric contexts, it is extremely useful a shape parametrization technique, associating the deformations to some numerical parameters, in order to enable some advanced algorithms — e.g. shape optimization, approximation of the parametric solution manifold, reduced order modeling techniques.

PyGeM is an open source Python package which implements advanced 3D geometrical parametrization and deformation techniques such as free form deformation (FFD) [1], radial basis functions (RBF) interpolation [2], inverse distance weighting (IDW) [3–5], and user defined custom deformations. Moreover it is able to interact with a vast range of mesh and geometry file commonly used both in academia and in industry. The complete list is the following:

- Computer Aided Design files (in .iges, .step, and .stl formats);
- mesh files (in .unv, Elmer, and OpenFOAM formats);
- output files (in .vtk format);
- LS-Dyna Keyword files (.k format).

Moreover, it is possible to apply the deformations to the points contained into a generic numpy `.ndarray`, extending further the applicability of such software.

The complete workflow describing the usage of the PyGeM package is illustrated in Fig. 1. After importing the mesh coordinates or, for the CAD files, the control points coordinates, we can select the desired parametrization technique, and the corresponding parameters. The user can also define a custom deformation. The numerical parameters whose control the deformation can be set directly within the code or parsing

a simple formatted text file, allowing for an easy integration in many existing frameworks. Finally the morphed object can be exported into the original file format. In Fig. 2 we show two demonstrative examples of geometric files which have been deformed by using PyGeM. The entire workflow can be implemented by the end user in few lines of code, thanks to the object oriented paradigm, which allows to maintain the interface clean and intuitive and encapsulate the algorithmic core within hierarchical classes.

The package is distributed with several tutorials that show its capabilities tackling the most common use cases. Additionally, an online documentation is provided [6].

2. The impact to research fields

A diverse range of numerical simulations made use of this geometrical morphing package, especially for parametric studies in the context of reduced order methods [7–9]. In the biomedical field we cite [10,11] where they employ RBF interpolation. In the naval field FFD has gained lots of attention thanks for its application to CAD files, for example in shape optimization studies [12–17], or in the context of isogeometric analysis [18]. For nautical application we mention [19], while for a benchmark CFD application see [20], where they also perform a reduction of the FFD parameters. The package has been successfully adopted also in automotive engineering, for example in [21,22].

3. The impact to industrial collaborations

PyGeM has been involved in several industrial collaborations and projects, matching the demand of an intuitive, easily integrable tool

for shape parametrization. In the Higher Education and Development programme, of the European Social Fund, it was exploited during the collaboration with Fincantieri S.p.A. within a shape optimization procedure developed to improve the hull shape of cruise vessels. Thanks to the numerical parametrization of the ship, it was in fact possible to feed the optimization algorithm in a completely automated fashion and, starting from the initial shape, converge to the geometrical configuration which minimizes the total resistance. The overall efficiency of the optimization cycles were further improved through the application of reduced order modeling techniques which significantly accelerated the simulations.

Further applications of PyGeM to industrial problems have been carried out in the context of the projects Underwater Blue Efficiency (UBE) and Seakeeping of Planing Hull Yachts (SOPHYA). Both projects have been funded by the Friuli Venezia Giulia regional government by means of the European Regional Development Fund and involve both academic and industrial partners such as Università di Trieste, Monte Carlo Yachts S.p.A. and MICAD s.r.l. The focus of both projects has been the overall hydrodynamic design of a motor yacht hull, and the detailed study of specific components such as underwater exhaust outlets. In such framework, PyGeM was used to deform the hull CAD geometry, and to parametrize the underwater exhaust outlet scoops. In addition, RBF algorithms have been used to extend the resulting CAD surface modifications to the surrounding volume and adjust accordingly the computational grids for the fluid dynamic simulations involved in the project. Again, this resulted in the possibility to run fully automated optimization cycles for the design of the full hull or its components.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

We thank our colleagues and research partners who contributed in the former and current developments of PyGeM library.

This work was partially supported by an industrial Ph.D. grant sponsored by Fincantieri S.p.A. (IRONTH Project), Italy, partially funded by the project UBE2 - "Underwater blue efficiency 2" funded by Regione FVG, Italy, POR-FESR 2014–2020, Piano Operativo Regionale Fondo Europeo per lo Sviluppo Regionale, Italy, and also partially funded 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.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.simpa.2020.100047>.

References

- [1] T.W. Sederberg, S.R. Parry, Free-form deformation of solid geometric models, in: *Proceedings of SIGGRAPH - Special Interest Group on GRAPHics and Interactive Techniques*, SIGGRAPH, 1986, pp. 151–159.
- [2] M.D. Buhmann, *Radial basis functions: theory and implementations*, vol. 12, Cambridge university press, 2003.
- [3] D. Shepard, A two-dimensional interpolation function for irregularly-spaced data, in: *Proceedings-1968 ACM National Conference*, ACM, 1968, pp. 517–524.
- [4] J.A.S. Witteveen, H. Bijl, Explicit mesh deformation using inverse distance weighting interpolation, in: *19th AIAA Computational Fluid Dynamics*, AIAA, 2009.
- [5] F. Ballarin, A. D'Amario, S. Perotto, G. Rozza, A pod-selective inverse distance weighting method for fast parametrized shape morphing, *Int. J. Num. Meth. Eng.* 117 (8) (2018) 860–884, <http://dx.doi.org/10.1002/nme.5982>.
- [6] PyGeM Documentation, <http://mathlab.github.io/PyGeM/>, (Accessed: 2020-10-20).
- [7] G. Rozza, M.W. Hess, G. Stabile, M. Tezzele, F. Ballarin, in: P. Benner, S. Griwet-Talocia, A. Quarteroni, G. Rozza, W.H.A. Schilders, L.M. Silveira (Eds.), *Basic Ideas and Tools for Projection-Based Model Reduction of Parametric Partial Differential Equations*, in: *Handbook on Model Order Reduction*, 2, De Gruyter, 2020, In Press.
- [8] F. Salmoiraghi, F. Ballarin, G. Corsi, A. Mola, M. Tezzele, G. Rozza, Advances in geometrical parametrization and reduced order models and methods for computational fluid dynamics problems in applied sciences and engineering: Overview and perspectives, in: *ECCOMAS Congress 2016 - Proceedings of the 7th European Congress on Computational Methods in Applied Sciences and Engineering*, vol. 1, 2016, Crete, Greece, pp. 1013–1031, [doi:10.7712/100016.1867.8680](https://doi.org/10.7712/100016.1867.8680).
- [9] G. Rozza, M.H. Malik, N. Demo, M. Tezzele, M. Girfoglio, G. Stabile, A. Mola, Advances in Reduced Order Methods for Parametric Industrial Problems in Computational Fluid Dynamics, in: R. Owen, R. de Borst, J. Reese, P. Chris (Eds.), *ECCOMAS ECFD 7 - Proceedings of 6th European Conference on Computational Mechanics (ECCM 6) and 7th European Conference on Computational Fluid Dynamics (ECFD 7)*, Glasgow, UK, 2018, pp. 59–76.
- [10] Z. Jiang, O. Mayeur, L. Patrouix, D. Cirette, J.-F. Witz, J. Dumont, M. Brieu, Patient-specific modeling of pelvic system from MRI for numerical simulation: Validation using a physical model, in: *International Conference on Medical Image Computing and Computer-Assisted Intervention*, Springer, 2019, pp. 19–30.
- [11] M. Tezzele, F. Ballarin, G. Rozza, Combined parameter and model reduction of cardiovascular problems by means of active subspaces and POD-Galerkin methods, in: D. Boffi, L.F. Pavarino, G. Rozza, S. Scacchi, C. Vergara (Eds.), *Mathematical and Numerical Modeling of the Cardiovascular System and Applications*, in: SEMA-SIMAI Series, 16, Springer International Publishing, 2018, pp. 185–207, http://dx.doi.org/10.1007/978-3-319-96649-6_8.
- [12] M. Tezzele, F. Salmoiraghi, A. Mola, G. Rozza, Dimension reduction in heterogeneous parametric spaces with application to naval engineering shape problems, *Adv. Model. Simul. Eng. Sci.* 5 (1) (2018) 25, <http://dx.doi.org/10.1186/s40323-018-0118-3>.
- [13] N. Demo, M. Tezzele, G. Gustin, G. Lavini, G. Rozza, Shape optimization by means of proper orthogonal decomposition and dynamic mode decomposition, in: *Technology and Science for the Ships of the Future: Proceedings of NAV 2018: 19th International Conference on Ship & Maritime Research*, IOS Press, 2018, pp. 212–219, <http://dx.doi.org/10.3233/978-1-61499-870-9-212>.
- [14] N. Demo, M. Tezzele, A. Mola, G. Rozza, An efficient shape parametrisation by free-form deformation enhanced by active subspace for hull hydrodynamic ship design problems in open source environment, in: *Proceedings of ISOPE 2018: The 28th International Ocean and Polar Engineering Conference*, vol. 3, 2018, pp. 565–572.
- [15] N. Demo, M. Tezzele, A. Mola, G. Rozza, A complete data-driven framework for the efficient solution of parametric shape design and optimisation in naval engineering problems, in: R. Bensow, J. Ringsberg (Eds.), *Proceedings of MARINE 2019: VIII International Conference on Computational Methods in Marine Engineering*, 2019, pp. 111–121.
- [16] M. Tezzele, N. Demo, G. Rozza, Shape optimization through proper orthogonal decomposition with interpolation and dynamic mode decomposition enhanced by active subspaces, in: R. Bensow, J. Ringsberg (Eds.), *Proceedings of MARINE 2019: VIII International Conference on Computational Methods in Marine Engineering*, 2019, pp. 122–133.
- [17] M. Tezzele, N. Demo, M. Gadalla, A. Mola, G. Rozza, Model order reduction by means of active subspaces and dynamic mode decomposition for parametric hull shape design hydrodynamics, in: *Technology and Science for the Ships of the Future: Proceedings of NAV 2018: 19th International Conference on Ship & Maritime Research*, IOS Press, 2018, pp. 569–576, <http://dx.doi.org/10.3233/978-1-61499-870-9-569>.
- [18] F. Garotta, N. Demo, M. Tezzele, M. Carraturo, A. Reali, G. Rozza, Reduced order isogeometric analysis approach for PDEs in parametrized domains, in: M. D'Elia, M. Gunzburger, G. Rozza (Eds.), *Quantification of Uncertainty: Improving Efficiency and Technology: QUIET Selected Contributions*, in: *Lecture Notes in Computational Science and Engineering*, 137, Springer International Publishing, Cham, 2020, pp. 153–170, http://dx.doi.org/10.1007/978-3-030-48721-8_7.
- [19] M. Tezzele, N. Demo, A. Mola, G. Rozza, An integrated data-driven computational pipeline with model order reduction for industrial and applied mathematics, in: *Special Volume ECMI*, 2020, In Press.
- [20] N. Demo, M. Tezzele, 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) (2019) 873–881, <http://dx.doi.org/10.1016/j.crme.2019.11.012>.
- [21] M. Bergmann, A. Ferrero, A. Iollo, E. Lombardi, A. Scardigli, H. Telib, A zonal Galerkin-free POD model for incompressible flows, *J. Comput. Phys.* 352 (2018) 301–325.
- [22] F. Salmoiraghi, A. Scardigli, H. Telib, G. Rozza, Free-form deformation, mesh morphing and reduced-order methods: enablers for efficient aerodynamic shape optimisation, *Int. J. Comput. Fluid Dyn.* 32 (4–5) (2018) 233–247, <http://dx.doi.org/10.1080/10618562.2018.1514115>.