



HAL
open science

Tamaas: a library for elastic-plastic contact of periodic rough surfaces

Lucas Frérot, Guillaume Anciaux, Valentine Rey, Son Pham-Ba,
Jean-François Molinari

► **To cite this version:**

Lucas Frérot, Guillaume Anciaux, Valentine Rey, Son Pham-Ba, Jean-François Molinari. Tamaas: a library for elastic-plastic contact of periodic rough surfaces. *Journal of Open Source Software*, 2020, 5 (51), pp.2121. 10.21105/joss.02121 . hal-04116934

HAL Id: hal-04116934

<https://hal.science/hal-04116934>

Submitted on 5 Jun 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Tamaas: a library for elastic-plastic contact of periodic rough surfaces

Lucas Frérot^{1, 2}, Guillaume Anciaux¹, Valentine Rey³, Son Pham-Ba¹, and Jean-François Molinari¹

1 Civil Engineering Institute, École Polytechnique Fédérale de Lausanne, Switzerland **2** Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland, United States. **3** Université de Nantes Sciences et Techniques, Nantes, France

DOI: [10.21105/joss.02121](https://doi.org/10.21105/joss.02121)

Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

Editor: [Kevin M. Moerman](#) ↗

Reviewers:

- [@likask](#)
- [@agshvarts](#)
- [@srmnitc](#)
- [@chennachaos](#)

Submitted: 06 February 2020

Published: 28 July 2020

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

Summary

Physical phenomena that happen at solid contact interfaces, such as friction and wear, are largely entwined with the roughness of the surfaces in contact. For example, the fact that the friction force between two solids in contact is independent of their apparent contact area is due to roughness, as the solids are only in contact over a smaller “true contact area” which only depends on the normal force (Archard, 1957). Roughness occurs on most man-made and natural surfaces (Persson, Albohr, Tartaglino, Volokitin, & Tosatti, 2005) and can span many orders of magnitude, from the nanometer scale to the kilometer scale (Renard, Candela, & Bouchaud, 2013). This poses a serious challenge to conventional numerical approaches in solid mechanics such as the finite-element method (FEM).

Boundary integral methods (Bonnet, 1995) are commonly employed in place of the FEM for rough elastic contact because of an inherent dimensionality reduction: the computational effort is focused on the contact interface whereas the FEM requires discretization of the volume of the solids in contact. In addition, the use of a half-space geometry provides a translational invariance: the computation of periodic equilibrium solutions can then be accelerated with the fast-Fourier Transform (Stanley & Kato, 1997).

However, because of the roughness, the total contact load is distributed over a small area and local contact pressures are expected to cause non-linear material behavior, such as plasticity. In this case, volume integral methods can be employed to account for plastic deformation (Telles & Brebbia, 1979). These enjoy properties analogous to boundary integral methods and can also be accelerated with a Fourier approach (Frérot et al., 2019b).

Taking plasticity into account is necessary in the accurate description of contact interfaces for the understanding of friction and wear. Moreover, high performance implementations are needed to model realistic rough surfaces with roughness spanning many orders of magnitude in scale.

Tamaas is a C++ library with a Python interface (Jakob, Rhineland, & Moldovan, 2017), developed in the [Computational Solid Mechanics Laboratory](#) at EPFL, that implements a unique Fourier-accelerated volume integral formulation of equilibrium (Frérot et al., 2019b) for the solution of elastic-plastic rough contact problems. The use of C++ allows for a particular focus on performance: most loops are parallelized using Thrust/OpenMP and the fast-Fourier transforms are computed with FFTW3/OpenMP. Thanks to this, it can handle simulations with upwards of 100 million degrees of freedom on a single compute node (Frérot et al., 2019b). Tamaas is aimed at researchers and practitioners wishing to compute realistic contact solutions for the study of interface phenomena.

Features and Performance

Tamaas provides access in its Python API to random rough surface generation procedures (e.g. Hu & Tonder (1992)), statistical tools (e.g. autocorrelation and power spectrum computations) and a variety of contact algorithms:

- Normal and adhesive contact schemes based on the conjugate gradient (Polonsky & Keer, 1999; Rey, Anciaux, & Molinari, 2017) and using the boundary integral method;
- Associated frictional contact using proximal algorithms (Condat, 2012);
- Elastic-plastic contact using the Fourier-accelerated volume integral method (Frérot et al., 2019b) and saturated surface pressure (Almqvist, Sahlin, Larsson, & Glavatskih, 2007).

We are not aware of any public software package providing implementation to all of the above methods, although the web-based package [contact.engineering](#) allows elastic normal contact solutions using a boundary integral method as well.

Tamaas also exposes in its Python API the accelerated linear operators it uses to compute equilibrium solutions, making prototyping new algorithms convenient.

We compare in figure 1 the scaling properties of Tamaas to a reference high-performance C++ FEM implementation named [Akantu](#) (Richart & Molinari, 2015) which uses the direct solver [MUMPS](#). The reference problem is the elastic equilibrium of a half-space with an isotropic spherical inclusion (Mindlin & Cheng, 1950), which is computed in serial for both implementations. N represents the number of points in the computational domain. For large N , Tamaas is two orders of magnitude faster than Akantu.

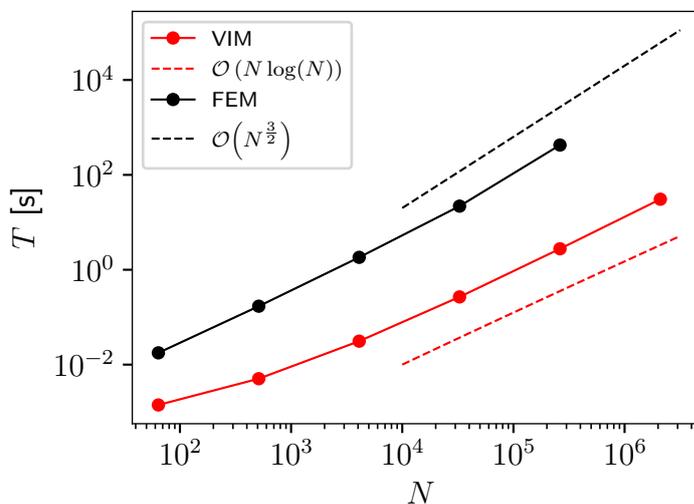


Figure 1: Scaling comparison between the accelerated volume integral method implemented in Tamaas and a finite-element method with a direct solver for the solution of the equilibrium of a half-space with a spherical isotropic inclusion. N is the number of points in the computational domain. When $N = 2^{18}$ Tamaas is 200 times faster than the FEM implementation Akantu.

Figure 2 shows the sub-surface plastic zones in a rough contact simulation, with color indicating their depth. The Fourier-accelerated approach allows an unprecedented level of detail on the topography of the zones which can have an influence on friction and wear (Frérot et al., 2019a).

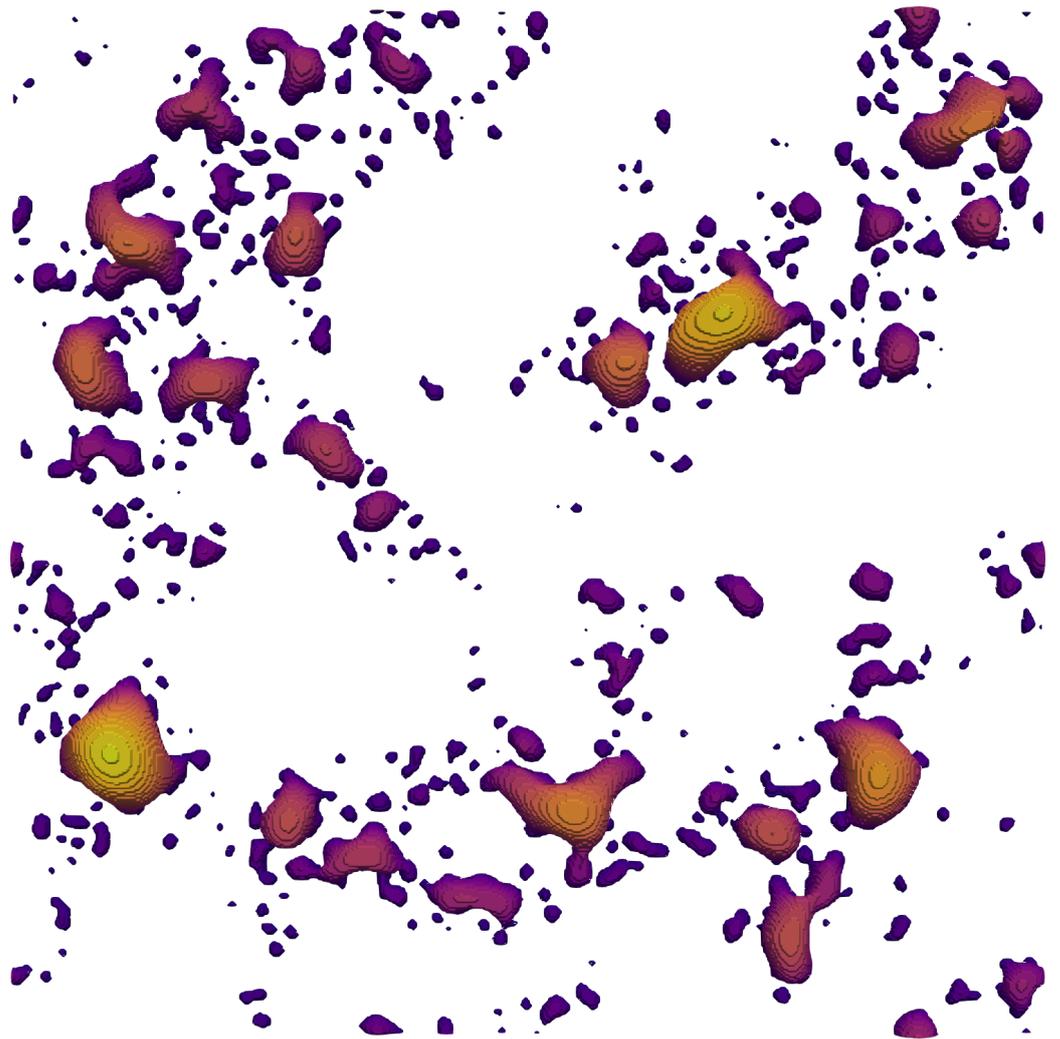


Figure 2: Sub-surface plastic zones in an elastic-plastic rough contact simulation. Lighter shades are zones deeper below the contact interface. The simulation used to produce this picture had more than 100 million degrees of freedom and ran on a single compute node (2×14 Intel Broadwell cores + 128GB RAM).

The following publications have been made possible with Tamaas:

- Yastrebov, Anciaux, & Molinari (2012)
- Yastrebov, Anciaux, & Molinari (2014)
- Yastrebov, Anciaux, & Molinari (2015)
- Yastrebov et al. (2017a)
- Yastrebov et al. (2017b)
- Rey et al. (2017)
- Rey & Bleyer (2018)
- Rey, Krumscheid, & Nobile (2019)
- Frérot, Aghababaei, & Molinari (2018)
- Frérot et al. (2019b)
- Frérot et al. (2019a)
- Brink, Frérot, & Molinari (2020)

Acknowledgements

We acknowledge the financial support of the Swiss National Science Foundation (grants #162569 “Contact mechanics of rough surfaces” and #191720 “Tribology of Polymers: from Atomistic to Continuum Scales”).

References

- Almqvist, A., Sahlin, F., Larsson, R., & Glavatskih, S. (2007). On the dry elasto-plastic contact of nominally flat surfaces. *Tribology International*, 40(4), 574–579. doi:[10.1016/j.triboint.2005.11.008](https://doi.org/10.1016/j.triboint.2005.11.008)
- Archard, J. F. (1957). Elastic deformation and the laws of friction. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 243(1233), 190–205. doi:[10.1098/rspa.1957.0214](https://doi.org/10.1098/rspa.1957.0214)
- Bonnet, M. (1995). *Boundary integral equation methods for solids and fluids*. Chichester ; New York: J. Wiley. ISBN: [978-0-471-97184-9](https://www.wiley.com/9780471971849)
- Brink, T., Frérot, L., & Molinari, J.-F. (2020). A parameter-free mechanistic model of the adhesive wear process of rough surfaces in sliding contact. *arXiv:2004.00559 [physics]*. Retrieved from <http://arxiv.org/abs/2004.00559>
- Condat, L. (2012). A PrimalDual Splitting Method for Convex Optimization Involving Lipschitzian, Proximable and Linear Composite Terms. *Journal of Optimization Theory and Applications*, 158(2), 460–479. doi:[10.1007/s10957-012-0245-9](https://doi.org/10.1007/s10957-012-0245-9)
- Frérot, L., Aghababaei, R., & Molinari, J.-F. (2018). A mechanistic understanding of the wear coefficient: From single to multiple asperities contact. *Journal of the Mechanics and Physics of Solids*, 114, 172–184. doi:[10.1016/j.jmps.2018.02.015](https://doi.org/10.1016/j.jmps.2018.02.015)
- Frérot, L., Anciaux, G., & Molinari, J.-F. (2019a). Crack Nucleation in the Adhesive Wear of an Elastic-Plastic Half-Space. *arXiv:1910.05163 [cond-mat]*. Retrieved from <http://arxiv.org/abs/1910.05163>
- Frérot, L., Bonnet, M., Molinari, J.-F., & Anciaux, G. (2019b). A Fourier-accelerated volume integral method for elastoplastic contact. *Computer Methods in Applied Mechanics and Engineering*, 351, 951–976. doi:[10.1016/j.cma.2019.04.006](https://doi.org/10.1016/j.cma.2019.04.006)
- Hu, Y. Z., & Tonder, K. (1992). Simulation of 3-D random rough surface by 2-D digital filter and fourier analysis. *International Journal of Machine Tools and Manufacture*, 32(1-2), 83–90. doi:[10.1016/0890-6955\(92\)90064-N](https://doi.org/10.1016/0890-6955(92)90064-N)
- Jakob, W., Rhineland, J., & Moldovan, D. (2017). Pybind11 – seamless operability between c++11 and python.
- Mindlin, R. D., & Cheng, D. H. (1950). Thermoelastic Stress in the Semi-Infinite Solid. *Journal of Applied Physics*, 21(9), 931–933. doi:[10.1063/1.1699786](https://doi.org/10.1063/1.1699786)
- Persson, B. N. J., Albohr, O., Tartaglino, U., Volokitin, A. I., & Tosatti, E. (2005). On the nature of surface roughness with application to contact mechanics, sealing, rubber friction and adhesion. *Journal of Physics: Condensed Matter*, 17(1), R1. doi:[10.1088/0953-8984/17/1/R01](https://doi.org/10.1088/0953-8984/17/1/R01)
- Polonsky, I. A., & Keer, L. M. (1999). A numerical method for solving rough contact problems based on the multi-level multi-summation and conjugate gradient techniques. *Wear*, 231(2), 206–219. doi:[10.1016/S0043-1648\(99\)00113-1](https://doi.org/10.1016/S0043-1648(99)00113-1)

- Renard, F., Candela, T., & Bouchaud, E. (2013). Constant dimensionality of fault roughness from the scale of micro-fractures to the scale of continents. *Geophysical Research Letters*, 40(1), 83–87. doi:[10.1029/2012GL054143](https://doi.org/10.1029/2012GL054143)
- Rey, V., Anciaux, G., & Molinari, J.-F. (2017). Normal adhesive contact on rough surfaces: Efficient algorithm for FFT-based BEM resolution. *Computational Mechanics*, 1–13. doi:[10.1007/s00466-017-1392-5](https://doi.org/10.1007/s00466-017-1392-5)
- Rey, V., & Bleyer, J. (2018). Stability analysis of rough surfaces in adhesive normal contact. *Computational Mechanics*, 1–13. doi:[10.1007/s00466-018-1556-y](https://doi.org/10.1007/s00466-018-1556-y)
- Rey, V., Krumscheid, S., & Nobile, F. (2019). Quantifying uncertainties in contact mechanics of rough surfaces using the multilevel Monte Carlo method. *International Journal of Engineering Science*, 138, 50–64. doi:[10.1016/j.ijengsci.2019.02.003](https://doi.org/10.1016/j.ijengsci.2019.02.003)
- Richart, N., & Molinari, J. F. (2015). Implementation of a parallel finite-element library: Test case on a non-local continuum damage model. *Finite Elements in Analysis and Design*, 100, 41–46. doi:[10.1016/j.finel.2015.02.003](https://doi.org/10.1016/j.finel.2015.02.003)
- Stanley, H. M., & Kato, T. (1997). An FFT-Based Method for Rough Surface Contact. *Journal of Tribology*, 119(3), 481–485. doi:[10.1115/1.2833523](https://doi.org/10.1115/1.2833523)
- Telles, J. C. F., & Brebbia, C. A. (1979). On the application of the boundary element method to plasticity. *Applied Mathematical Modelling*, 3(6), 466–470. doi:[10.1016/S0307-904X\(79\)80030-X](https://doi.org/10.1016/S0307-904X(79)80030-X)
- Yastrebov, V. A., Anciaux, G., & Molinari, J.-F. (2012). Contact between representative rough surfaces. *Physical Review E*, 86(3). doi:[10.1103/PhysRevE.86.035601](https://doi.org/10.1103/PhysRevE.86.035601)
- Yastrebov, V. A., Anciaux, G., & Molinari, J.-F. (2014). The Contact of Elastic Regular Wavy Surfaces Revisited. *Tribology Letters*, 56(1), 171–183. doi:[10.1007/s11249-014-0395-z](https://doi.org/10.1007/s11249-014-0395-z)
- Yastrebov, V. A., Anciaux, G., & Molinari, J.-F. (2015). From infinitesimal to full contact between rough surfaces: Evolution of the contact area. *International Journal of Solids and Structures*, 52, 83–102. doi:[10.1016/j.ijsolstr.2014.09.019](https://doi.org/10.1016/j.ijsolstr.2014.09.019)
- Yastrebov, V. A., Anciaux, G., & Molinari, J.-F. (2017a). On the accurate computation of the true contact-area in mechanical contact of random rough surfaces. *Tribology International*. doi:[10.1016/j.triboint.2017.04.023](https://doi.org/10.1016/j.triboint.2017.04.023)
- Yastrebov, V. A., Anciaux, G., & Molinari, J.-F. (2017b). The role of the roughness spectral breadth in elastic contact of rough surfaces. *Journal of the Mechanics and Physics of Solids*, 107, 469–493. doi:[10.1016/j.jmps.2017.07.016](https://doi.org/10.1016/j.jmps.2017.07.016)