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

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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, Rhinelander, & 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.

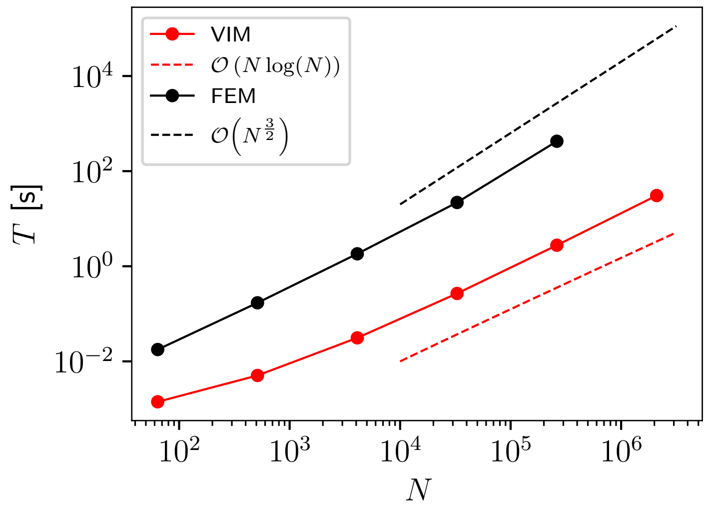

Figure 1: Scaling comparison between the acclerated volume integral method implemented in Tamaas and a finite-element method with a direct solver for the solution of the equilibrium of a half-space with a spherical isotropic inclusion. N is the number of points in the computational domain. When $N = 2^{18}$ 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 unprecendented level of detail on the topography of the zones which can have an influence on friction and wear (Frérot et al., 2019a).

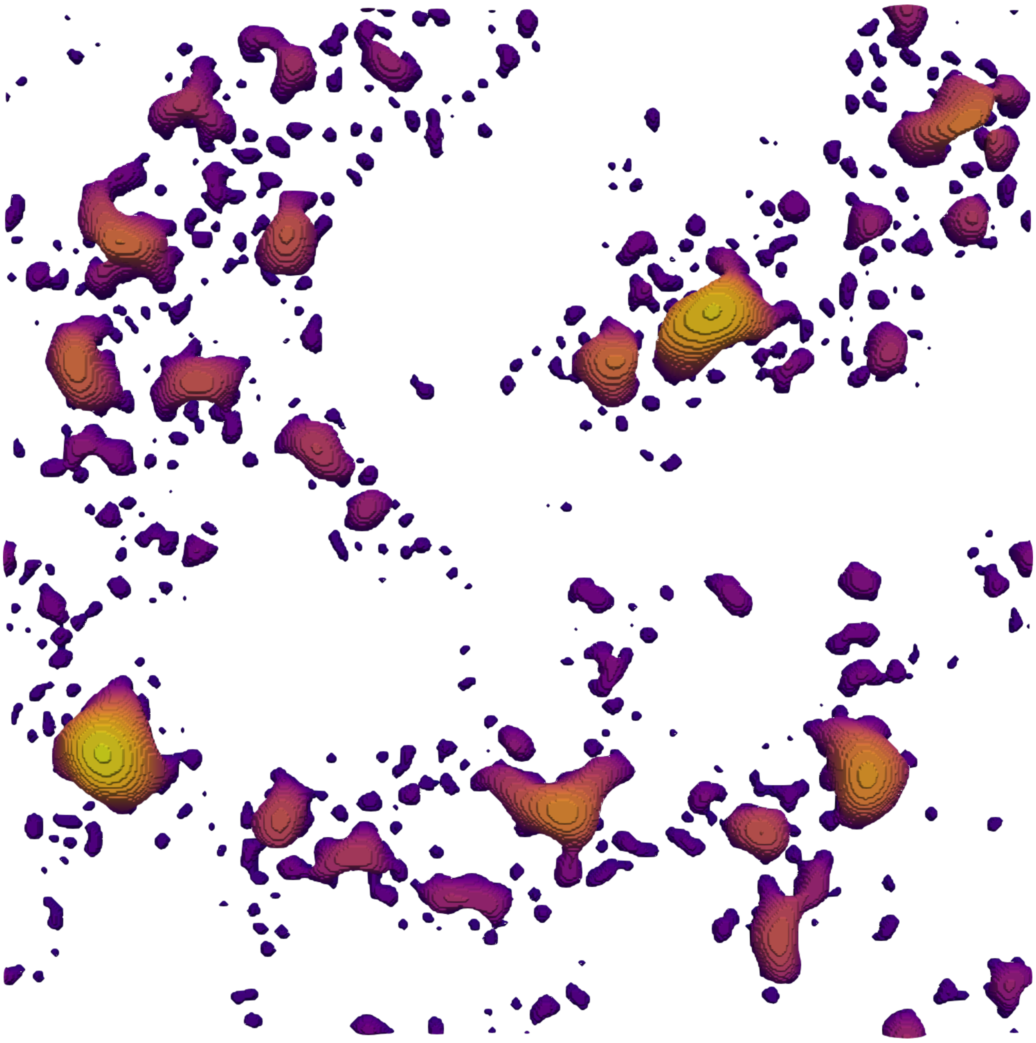

Figure 2: Sub-surface plastic zones in an elastic-plastic rough contact simulation. Lighter shades are zones deeper below the contact interface. The simulation used to produce this picture had more than 100 million degrees of freedom and ran on a single compute node (2×14 Intel Broadwell cores + 128GB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

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