



# Exploring the Use of Molecular Dynamics Simulations for High-Performance Space Debris Collision Modelling

## Executive Summary

**Authors:** Pablo Gómez<sup>1</sup>, Fabio Grati<sup>2</sup>

**Affiliation:** <sup>1</sup>ESA ACT, <sup>2</sup>Technical University Munich

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**Contacts:**

Fabio Grati

Tel: +49-89-289-18-168

e-mail: Email

Leopold Summerer (Technical Officer)

Tel: +31(0)715654192

Fax: +31(0)715658018

e-mail: [act@esa.int](mailto:act@esa.int)



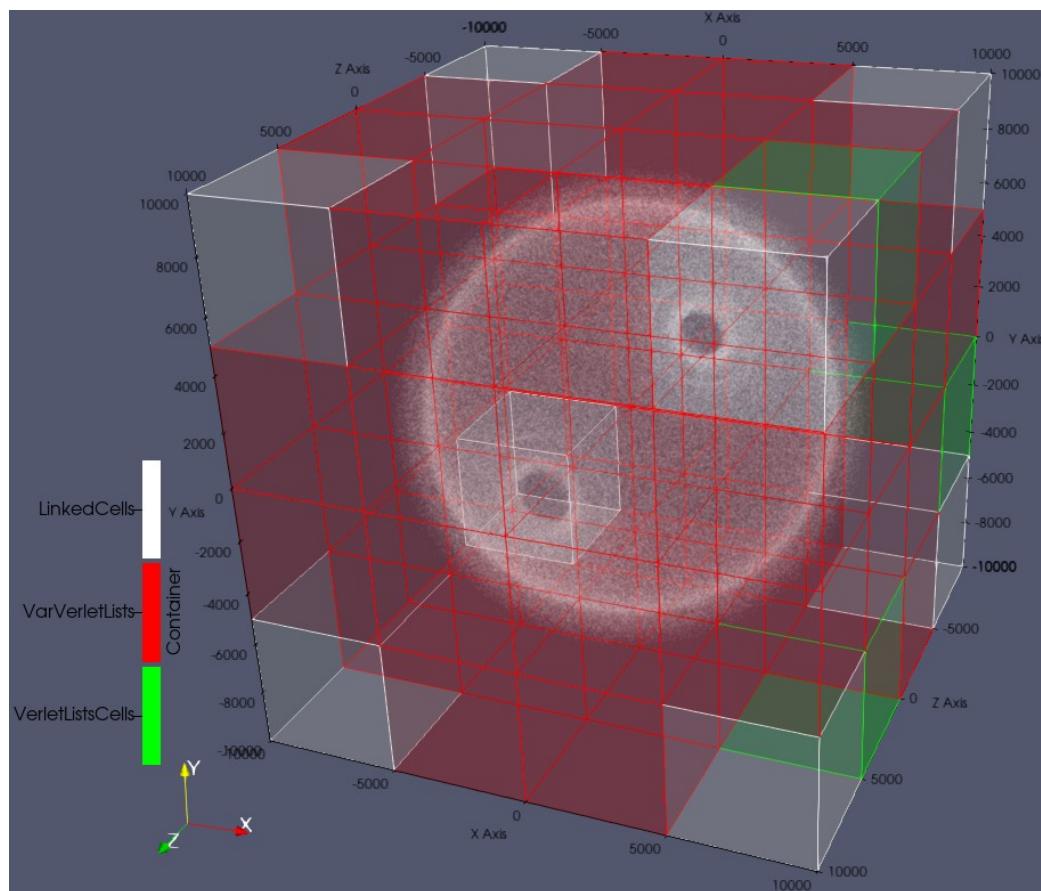
Available on the ACT website  
<http://www.esa.int/act>

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## Picture:



## Motivation:

Investigate the use of algorithmic improvements and high-performance computing for deterministic space debris collision simulations with small time-stepping and high collision fidelity in long-term simulations.

## Methodology:

For long-term studies, numerical simulations are at the center of predicting the space debris environment of the upcoming decades. In the scope of the study, we present the architecture and proof-of-concept results for a numerical simulation capable of modeling the long-term debris evolution over decades with a deterministic conjunction tracking model in contrast to typically employed Monte Carlo methods. For the simulation, an efficient propagator in modern C++ accounting for Earth's gravitational anomalies, solar radiation pressure, and atmospheric drag was developed. We utilized AutoPas, a sophisticated particle container, which automatically selects the most efficient data structures and algorithms. Using OpenMP and MPI, the simulation was scaled up to over 600 000 particles being simulated on up to 3584 cores in parallel.

## Results:

- Deterministic collision / conjunction modeling in long-term space debris simulations is feasible using high-performance computing methods, achieving 50x realtime on just 128 compute nodes for over 600 000 particles.
- Modeling the small debris environment (over 500 000 particles in LEO) becomes feasible with these simulations.
- Critical points for efficient simulations are: Highly parallel propagator with as large a timestep as numerically stable, efficient conjunction tracking with sub-timestep resolution and a smart domain decomposition (e.g. using polar coordinates).
- Observed conjunctions are highly reliant on the assumed size of objects, thus data quality is paramount for realistic simulations.

## Publications:

- Pablo Gómez, Fabio Gratl, Oliver Bösing, and Dario Izzo. "*Deterministic Conjunction Tracking in Long-term Space Debris Simulations*". In: Proceedings of the third IAA Conference on Space Situational Awareness (ICSSA) (2022).
- Jonas Schuhmacher. "*Efficient Implementation and Evaluation of the NASA Breakup Model in Modern C++*". Bachelor's Thesis, TUM, 2021.
- Oliver Bösing. "*Efficient Trajectory Modelling for Space Debris Evolution*". Bachelor's Thesis, TUM, 2021.
- Albert Noswitz. "*Modeling Upcoming Megaconstellations in Space Debris Environment Simulations*". Bachelor's Thesis, TUM, 2022.

## Highlights:

Following up we plan to investigate a polar coordinate-based domain decomposition as our results indicate great scaling potential that should allow even larger, long-term simulations e.g. on LRZ's SuperMUC.