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

Study reference number: 21-5105

Type of activity: Standard study (30k€)

Project Summary

Objective

Investigate the use of algorithmic improvements and high-performance computing to investigate deterministic space debris collision simulation with small time-stepping and high collision fidelity.

Target university partner competences

AutoPas, High Performance Computing, Availability of Large-scale Computational Power

ACT provided competences

Space Debris Modeling, Access to Space Debris Tools & Data

Keywords

Space Debris, Numerical Simulation, High Performance Computing

Study Objective

The increasing number of satellite launches poses challenges to space debris tracking, analysis and prediction. Current methods to simulate the evolution of space debris rely on Monte Carlo approaches to tackle the computational challenges of tracking a large number of possible collisions of space debris. The goal of this study is to create a deterministic collision simulation using recent high-performance computing (HPC) advances to tackle the computational costs. This should allow smaller time steps and higher simulation fidelity.

Background and Study Motivation

Recent years have seen a substantial increase in satellite launches. In 2020, for the first time, over a thousand objects were launched into low earth orbit [1] (see Fig. 1). Many of these launches immediately contribute to the space debris environment with, e.g., spent upper stages [2]. The debris concentration is further amplified by fragmentation events, such as explosions or collisions, which can create large numbers of small fragments [3] (see Fig. 2).

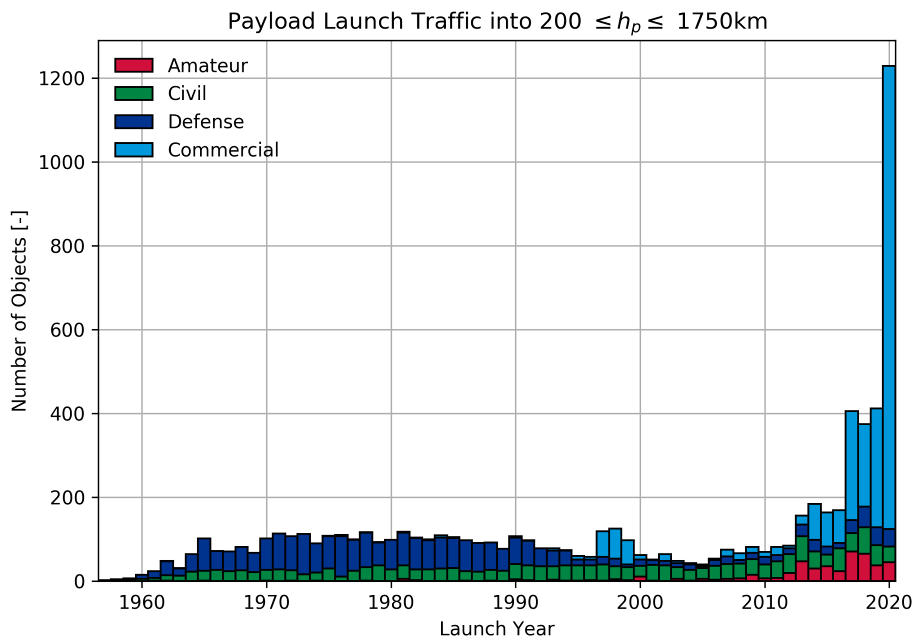

Figure 1 - Launches into low earth orbit per year [1]

Current statistical estimates put the number of debris objects at 128 million for objects between 1 mm and 1 cm, 900 000 for 1 cm to 10 cm and 34 000 for objects larger than 10 cms [4]. Space debris has become a central topic for space agencies [5] and ESA in particular, which has been pioneering this field with its Clean Space initiative and recently commissioned the first active debris removal mission [6].

ESA and other space agencies have developed a range of sophisticated tools to analyse and predict the evolution of the space debris as well as likely conjunction events of space debris and active spacecraft [7,8]. However, simulating thousands or millions of space debris particles over a time span of decades results in a large computational burden. Previous long-term models therefore use a semi-deterministic approach based on Monte Carlo methods to keep the computational costs tangible [9].

This study will explore an alternative route and aim to incorporate state-of-the-art techniques from HPC to achieve the necessary computational efficiency and scaling to create a simulation that relies on deterministic conjunction tracking instead. This bears the promise to combat the inherent variability of Monte Carlo simulations [10]. A deterministic approach has become conceivable now, as hardware and software to run petascale numerical simulations are available [11,12]. The study will rely on utilizing AutoPas [12], a software library for autotuned particle simulation, which has seen successful application in the context of molecular dynamics simulations [13-15].

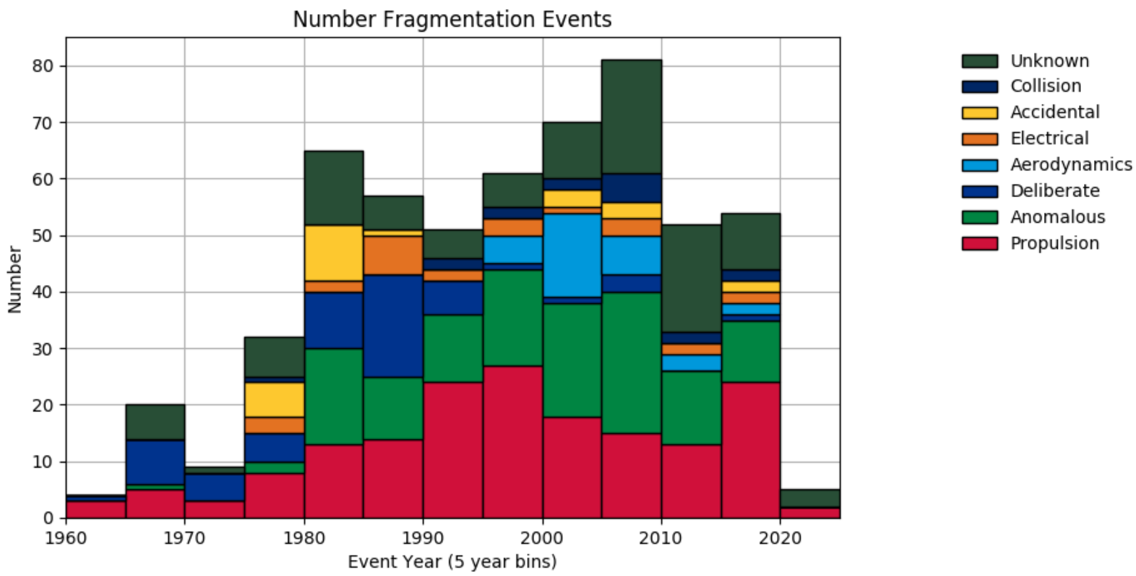

Figure 2 - Fragmentation events per year and type [1]

In summary, the goal will be to create a space debris particle simulation based on AutoPas with a deterministic conjunction event handling. The simulation will aim to simulate between 50 000 and 500 000 particles over a time span between 10 and 100 years. Several focus areas such as cloud fragmentation or long-term evolution are conceivable and will be investigated in detail.

Proposed Methodology

1. **WP 1 - Conceptual Design**
   Using the state of the art approaches, the main focus will be to define the requirements and derive the options for simulation design in regards to physical fidelity. Input to this phase will come from ESA, and in particular from ESA's Space Debris Office. This will result into an optimalily trade-off between physical fidelity and high computational efficiency.

2. **WP 2 - Soft- and Hardware Preparation**
   Using the results of WP 1, the availability of the necessary computational resources to run the planned large-scale simulations will be ensured. The computational infrastructure and the AutoPas library for a seamless integration with the proposed simulation will be prepared, including a detailed specification of the software and hardware environment for the simulation.

3. **WP 3 - High-level Prototyping**
   Based on the outcome from WP 1 and 2, ESA will implement a Python (or similar) prototype of the mathematical description of the dynamical system to serve as a baseline for future comparison. The prototype will be analysed in regards to fidelity and computational efficiency.

4. **WP 4 - HPC Implementation**
   This main WP of the study will implement a high-performance version of the high-level prototype, likely in C++ 17, focusing on optimizing the implementation to achieve maximal computational efficiency. Once confident in the accuracy and satisfied with the computational performance ESA will provide input on the technical aspects to set up the simulation's initial conditions.

5. **WP 5 - Simulation Runs**
   During this WP, the prepared simulations will run on the hardware requisitioned in Step 2.

6. **WP 6 – Outreach**
   Preparation of the final report and an open access publication of the results. Results may be presented at suitable conferences such as the *European Conference on Space Debris*.

Study plan

WP \ Step	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
1 - Conceptual Design									
2 - Soft- and Hardware Preparation									
3 - High-level Prototyping									
4 - HPC Implementation									
5 - Simulation Runs									
6 - Outreach									

Table 1 - Study plan; Activities by ESA in blue, the partner in orange and joint activities in green

ACT Contribution

The project will be conducted in close scientific collaboration with ESA researchers. In particular ESA researchers will provide technical expertise related to the space debris environment, space debris propagation and evolution, mathematical modelling of conjunction events, providing data for validation, and initialization of the created simulation

ESA plans to provide a prototypical implementation for computation of the necessary forces and simulation events in a high-level programming language such as Python. ESA will assist in optimising the high-performance implementation.

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