

Numerical Study of Ammonium Nitrate / Fuel Oil Detonations for Large Scale Pattern of Life Simulations

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ABSTRACT

Next generation frameworks have been developed to support large-scale pattern-of-life simulations. These simulations can be used to assess the consequences of hazardous events in urban environments and to develop effective emergency response strategies to these events. CAE has been prototyping large-scale pattern of life simulations in real time, human-in-the-loop operations for concept development, course of action analysis, and training. The simulation of bomb explosions is a critical component of emergency response simulations and provides valuable insight into the potential effects of an explosion on infrastructure and populations. This paper will report three simulation scenarios of Ammonium Nitrate/Fuel Oil (ANFO) explosions in urban areas of Tallinn, Estonia. The blasts were simulated with BlastFOAM, an inviscid compressible flow solver for high-explosive detonations and airblasts that integrates with OpenFOAM, a computational fluid dynamics (CFD) solver. Detonations ranging from 5 000 to 10 000 lbs of a fertilizer lorry in the areas of Tallinn's Kalevi Stadium, Town Square and Freedom Square were simulated. The simulations considered the variability of explosive charge, surrounding topology including buildings, infrastructure and terrain. The framework was integrated with detailed 3D urban geometry sourced from the Estonian Land Board. A 72-core virtual machine was used for meshing and running the CFD solver for up to 1 000 milliseconds of simulation time. The blast pressures were imported into the geospatial digital twin and could be visualized along with the spatial and temporal distributions of pressure data that were used to predict the probabilities of human casualties based on the pattern of life. The paper will demonstrate the effectiveness of using advanced frameworks and pattern-of-life simulations as a crucial tool for training emergency responders and evaluating the efficacy of response plans.

ABOUT THE AUTHORS

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INTRODUCTION

Over the last decades, numerical simulations have seen their usage increase extensively (Borrelli & Wellmann, 2019). This has seen the emergence of a variety of numerical tools that range from low to high fidelity, to respond to varying needs in accuracy. The field of Computational Fluid Dynamics (CFD) has seen a large increase in accuracy, techniques, and speed. The scale of the simulations has consistently increased with the improvement of computing complexes as well as more efficient methods (Abbas-Bayoumi & Becker, 2011). More recent developments have enabled multi-fluid compressible simulations that are suitable for large-scale urban environments (Drazin, 2017).

The advent of large-scale pattern of life simulations is becoming critical to the preparation and prevention of hazardous scenarios in urban environments. Such events cover a variety of operations, such as power outages, fire prevention and containment and explosive detonations. This paper presents the integration of high fidelity CFD simulations of detonations in a digital twin that includes pattern of life simulation. The objective is to provide accurate representation of the detonations and compute the impact on the population and when combined with the simulated pattern of life, based on location, time of day and any special events or gatherings.

The Pattern of Life framework is briefly described. The CFD simulation process is detailed, and the information extracted to the pattern of life framework is presented. Finally, two validation cases are presented to demonstrate how it can be integrated into a large-scale simulation. The impact of the detonation within the simulation is presented and finally, lessons learned are summarized in the conclusion.

PATTERN OF LIFE FRAMEWORK

Pattern of life simulations are a valuable tool for evaluating damages from large-scale explosions, especially in scenarios involving urban environments or critical infrastructure. By adding human population layers, transportation, and infrastructure elements, these simulations can provide insights into the potential impact and consequences of a detonation event. CAE has been prototyping large-scale pattern of life simulations in real time, human-in-the-loop operations for concept development, course of action analysis, and training. This new framework is scalable and simulates patterns of life at the country, city or street level and allows for visualization and interaction in an immersive, 3D environment. Figure 1 and Figure 2 show examples from the Pattern of Life framework. The framework combines a population activity model, a high-fidelity crowd simulation and infrastructure metadata. The developments

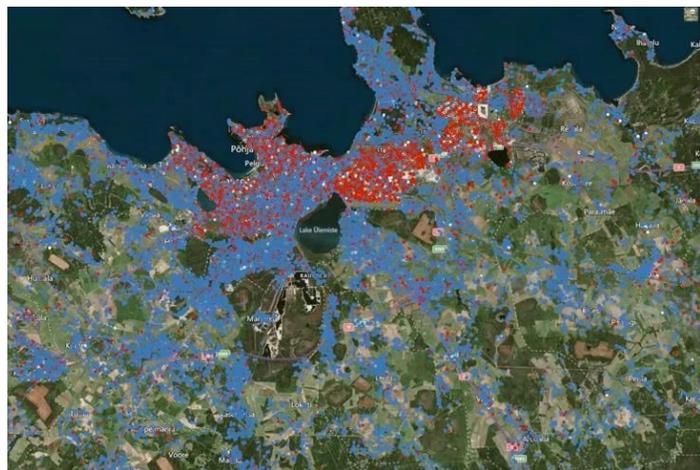


Figure 1. Population in and around Tallinn as simulated by the pattern of life. Blue and red dots represent ethnic Estonian and ethnic Russian population respectively.

discussed in this paper add external threat factors, such as detonation simulations, to the framework. This framework has previously been used to successfully demonstrate a civil resilience scenario involving a cyberattack on the London power network and a military course of action with ethnically motivated paramilitary operations and civil unrest (Giannias, et al., 2022).



Figure 2. Closeup view of Tallinn. Data for all buildings in Estonia are provided by the Estonian Land Board. White buildings are available at a lower resolution and detail. Old Town Tallinn, seen here as textured buildings in the center, are exact representations.

COMPUTATIONAL FLUID DYNAMICS SIMULATION

As part of this large-scale pattern of life simulation, CAE has investigated the use of Computational Fluid Dynamics to produce accurate blast patterns for various scenarios. The simulated blasts use an Ammonium Nitrate/Fuel Oil (ANFO) mixture. This explosive can be fabricated with relative ease and has a specific energy that allows its use in truck bomb scenarios. This explosive was used in the Oklahoma (Irving, 1995) and Oslo (Gimse, 2011) incidents.

The blasts were simulated using BlastFOAM, developed by Synthetik Applied Technologies inside the OpenFOAM framework (Heylmun, Vonk, Shields, & Brewer, 2022). It is an open-source application for compressible inviscid multi-fluid flow to be used in detonation cases (Stevens, Vonk, & Brewer, 2018). BlastFOAM includes a chemical reaction solver to accurately simulate the energy released by the explosive device. It was used to predict the propagation of the explosion in the two presented scenarios. The detonation simulations made extensive use of cloud computing technology on Microsoft Azure. The Fsv2-series virtual machines were used to solve for up to 1000 milliseconds of simulation time in each of the scenarios. The scalability of cloud resources permitted the use of F72s_v2 machines (72 cores, 144GB of RAM) for computation and F8s_v2 (8 cores, 16GB of RAM) machines for post-processing, utilizing the same hard drive to avoid time-consuming data transfer.

Blast Parameters

The BlastFOAM software suite offers many options to correctly simulate the multiple phases in the fluid domain (Heylmun, Vonk, Shields, & Brewer, 2022). Two solver phases are required: air and ANFO. The air phase is simulated as a constant ideal gas, meaning the air will not change its molecular properties as it is subjected to the ANFO reaction. The ANFO phase is simulated as a reactant material, with a reactant-product transition. The product parameters are based on the Jones-Wilkins-Lee (JWL) model (Lee, Hornig, & Kury, 1968). This commonly used model for such simulations describes the product of detonation in the principal terms A, B, C, R1, R2 and E0 for the equation of state parameters (Sanchidrian, Castedo, Lopez, Segarra, & Santos, 2015). Furthermore, BlastFOAM offers a variety of methods to control the activation of the reaction. In the scenarios studied, a simple linear activation method with a single fuse is used to detonate the explosive. The explosive charge is modeled as a sphere and is placed directly at the target location.

Geometry Preparation

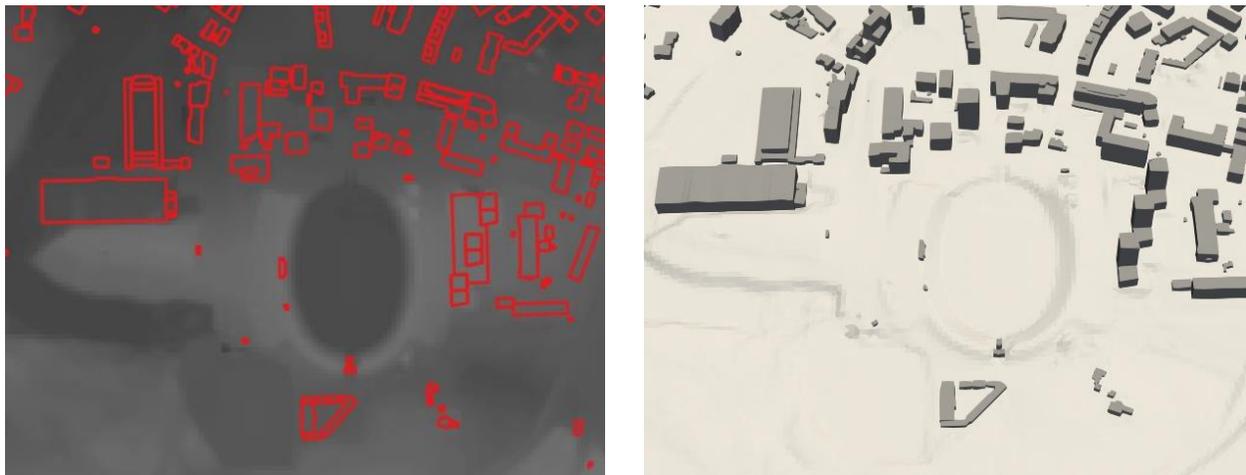


Figure 3. (Left) 2D footprint data for the buildings and (right) 3D buildings extracted on the terrain topography

To correctly correlate the CFD simulation with the pattern of life simulation, the same data source is used to generate the geometric model. The elevation geometry is first extracted from the digital elevation model (DEM). Then, buildings are generated using 2D footprint data, as seen in Figure 3. These footprints contain building height information at the displayed levels, which are used to generate the building's 3D footprint. Finally, the buildings' models are stitched to the terrain geometry to populate the simulation, as seen in the right image of Figure 3. This process ensures that the 3D geometry is watertight, which is required to correctly mesh and solve the fluid domain. The terrain model and building models are separated to minimize pre-processing and post-processing efforts.

A large area of the city of Tallinn was extracted as a single model to support the described scenarios, accounting for the estimated blast radius of the multi-ton detonations. The extracted database is then offset to center the detonation in the computational domain for each simulation. This process simplifies data post-processing by computing localized effects of the blast at the same origin, followed by a simple transformation to the appropriate latitude/longitude of the blast location.

Mesh Generation & Simulation

To improve simulation time, a coarse base mesh is created to integrate the city geometry into the CFD computational domain at low computational cost. An automatic mesh refinement (AMR) method is used to correctly resolve and follow the initial shockwave and subsequent high-pressure areas. The AMR uses the air density geometric gradient to determine which cells need to be refined, followed by an octree decomposition of the targeted cells. The refined mesh stabilizes the gradient by reducing dissipation caused by the mesh geometry.

Similarly, the simulation is resolved using an adaptative time step to ensure proper propagation of the shockwave in the fluid domain while maintaining solver stability. The solver scheme used requires a Courant-Friedrichs-Lewy (CFL) number below 0.5 to ensure stability. Due to the high velocities generated by the detonation and the small mesh sizes required to maintain the shockwave, the initial timesteps are very small (20 μ s) and steadily increase as the shockwave propagates and the cell velocity and size increases (reaching 30 μ s at the end of the simulation). A summary of the execution time is found in Table 1. The simulation is solved until the overpressure has diminished below the minimum threshold for damage (US Air Force, 2004), after which the subsequent time steps do not generate additional content for the life of pattern simulation.

Table 1 - Scenario Execution Time

Scenario	Execution Time (hours)	Execution Time (core-hours)	Max Number of Cells (millions)	Number of Timesteps (-)
Freedom Square	23.0	1652.7	1.99	39417
Stadium	21.7	1564.4	2.33	41574
Town Square	20.2	1453.4	1.60	39390

Post-Processing and Integration

The CFD simulation provides the maximum overpressure in the fluid domain. The maximum overpressure at ground and building level is extracted from the simulation results and used to generate a 2D map of the blast evolution. Overpressure contours are extracted at 0.5 psi, 2 psi and 10 psi. These levels were determined based on effects on the human body and their casualty rating, as described in (Zipf & Cashdollar, 2006), describing light, moderate, and widespread casualty ratings. The contours for each of the three different overpressure levels are processed into a GeoJSON format (Butler, et al., 2016), to be integrated by CAE's pattern of life simulation software. These overpressure contours generate closed loop polygons that can then be used to determine the population and infrastructure affected by the blast level. Figure 4 details the post-processing workflow.

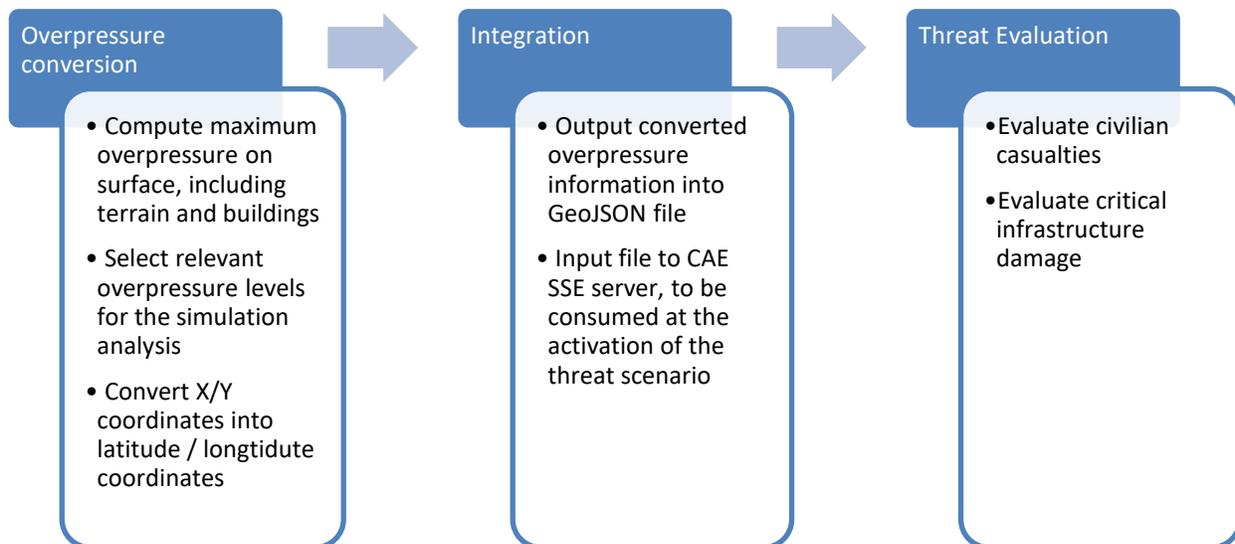


Figure 4. Workflow for processing BlastFOAM CFD simulation results into the pattern-of-life simulation

RESULTS

Three different scenarios were analyzed in this paper: a detonation near Tallinn's Town Square, the Kalevi Keskstaadion Stadium and Freedom Square. All scenarios feature ANFO explosives deployed using truck bombs.

Town Square

In the town square simulation, 5 000 lbs of ANFO explosive is detonated near the town square (Figure 5). The detonation location is highlighted with a blue arrow, as the truck is detonated on the neighboring street of the town square (orange circle).

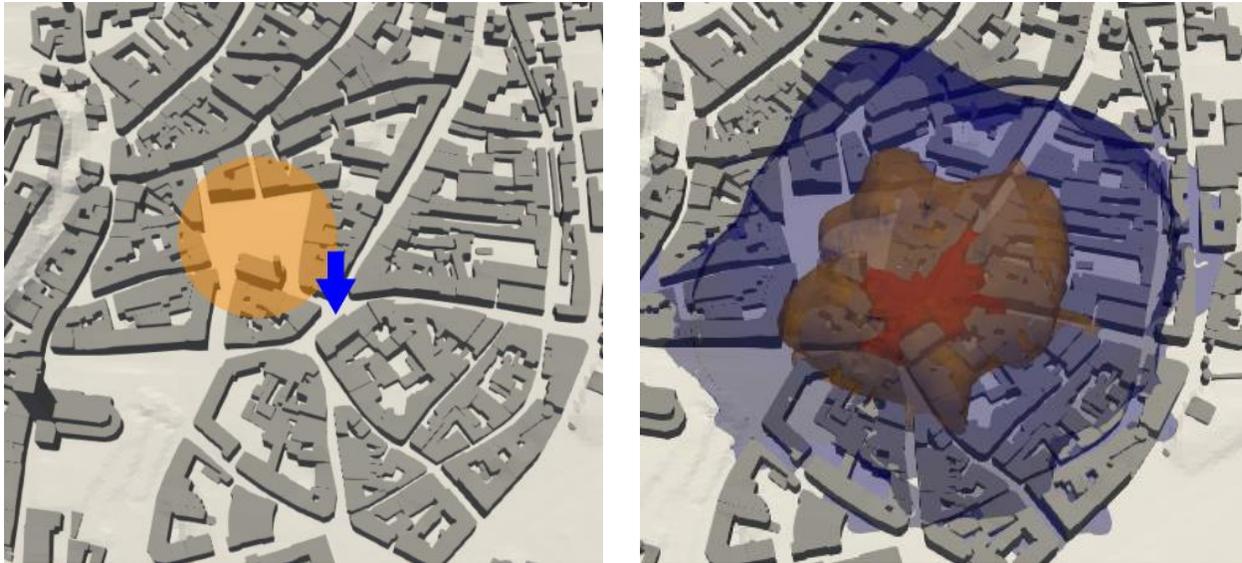


Figure 5. (Left) Town Square (orange circle) with the detonation location (blue arrow) and (right) Town Square 3D iso-contour of peak overpressure

The right image of Figure 5 shows the three iso-contour levels of interest, which are minimal injuries (blue, outer contour), moderate injuries (orange, mid contour) and widespread casualties (red, inner contour). The presence of narrow buildings near the detonation site greatly influences the shape of the high level of overpressure, containing it to the neighboring streets. As the blast propagates, the shockwave passes over the buildings and expands towards the town square. The lower overpressure iso-contour (in blue) is less influenced by the buildings, maintaining a more spherical shape.

Validation of the area of effect is done by comparing the radius of the detonation to empirical measurements (US Air Force, 2004). The approximate blast radius is extracted from the simulation using the ground peak overpressure by measuring the diameter at multiple orientations and computing their average. Table 2 summarizes the results for all levels measured. The highest overpressure level is significantly larger than the empirical measurement, however this could be influenced by the cross shaped street, which propagates and reflects the blast further through the narrow streets.

Once integrated, the peak overpressure levels can be used to calculate the potential impact on the population, as shown in Figure 6. Inside the highest overpressure level (10 psi), casualties approach 100%. At the middle level (2 psi), most civilians will suffer injuries and will require medical attention to be treated. Inside the lowest level (0.5 psi), while injuries are likely to be minor, they will still need attention. The simulation continuously calculates the number of potentially affected civilians, while simultaneously performing an evacuation that correctly accounts for their movement in the narrow streets of Old Town, Tallinn. In addition to civilian metadata, affected infrastructure can be evaluated as well. For example, buildings inside the 10-psi level will suffer severe damage and require emergency response accordingly. Note that building damage was not assessed as part of this effort. One of the benefits of the integrated digital twin is that critical infrastructure, such as hospitals, schools, police stations and government buildings, can be tagged to ascertain their capability to operate following the detonation.

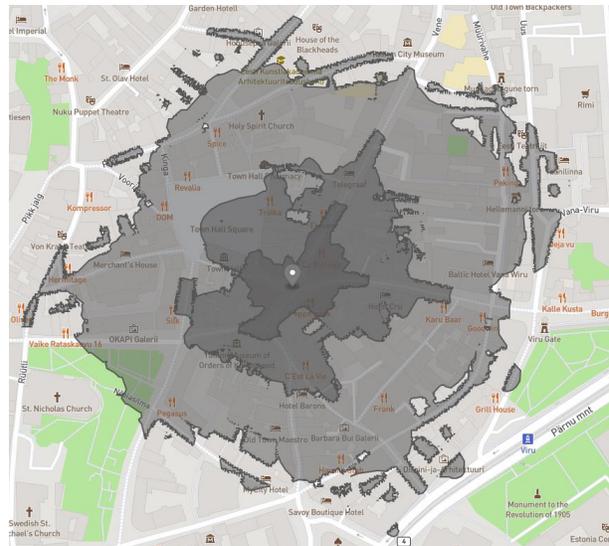


Figure 6. 2D map for the three peak overpressure levels extracted at ground level for the Town Square scenario

Table 2. Comparison of empirical distances to simulation results for the Town Square scenario

Peak Overpressure (psi)	Empirical Stand-off distance (ft)	Average Simulation Radius (ft)
0.5	913	708
2.0	314	372
10.0	93	188

Kalevi Kesksstaadion Stadium

In the Kalevi stadium simulation, a 10 000 lb ANFO explosive is detonated (Figure 7) in a neighboring parking lot (blue arrow), targeting the open-air stadium (orange oval). As opposed to the previous case, this scenario is situated in a much more open space and large solid infrastructure but with a high concentration of human activity in a confined area. The blast simulation shown in the right image of Figure 7 indicates a more spherical shape for all three iso-contours, set at the same overpressure values as the previous case. Nevertheless, the presence of the 3 tall buildings on the right of the detonation location contribute to reflect the blast energy towards the stadium.

The simulation is again validated against empirical measurements (US Air Force, 2004). Table 3 shows that the simulation results are in good agreement with the smaller overpressure iso-contour level. Here again, however, the medium and high overpressure levels are larger compared to empirical measurements. In this scenario, the detonation is in a relatively open space, so the energy dissipates more evenly in all directions. It is worth noting that the empirical measurements are based on TNT, so they may not hold well when compared to an ANFO detonation. When comparing both scenarios, the ANFO mass was converted into a TNT mass for the empirical measurement using the Relative

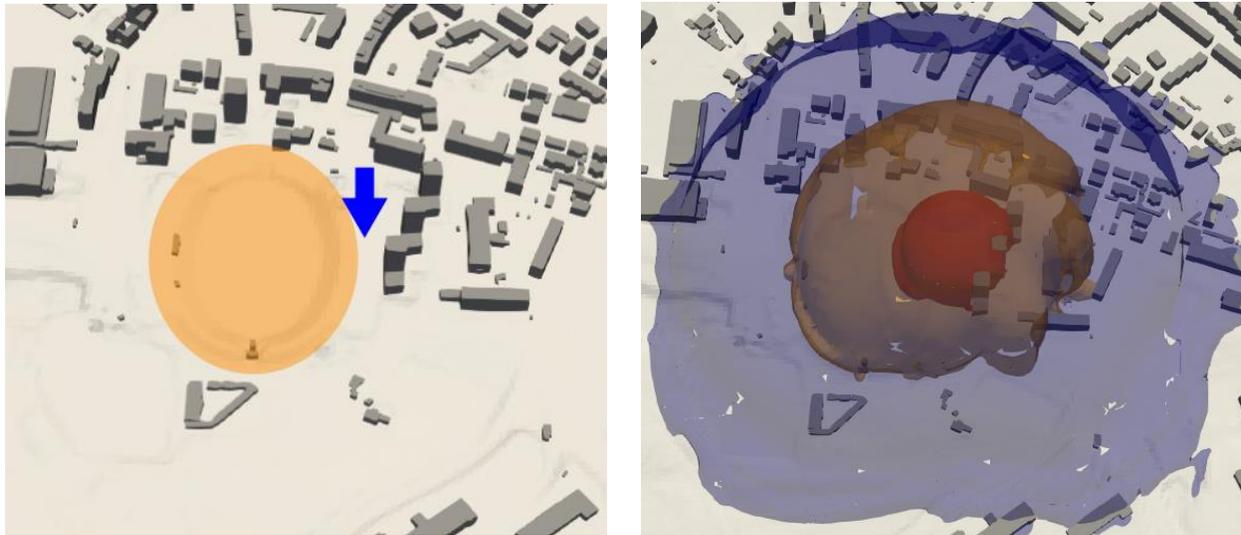


Figure 7. (Left) Kalevi Stadium (orange oval) with the detonation location (blue arrow) and (right) 3D iso-contour of peak over-pressure

Effectiveness factor (Surhone, Timpledon, & Marsseken, 2010). A comparison to a clinical simulation, without terrain and building effects would help to quantify the difference between the CFD simulation and the empirical measurements. Although the empirical and simulation results are not in agreement, the simulations produce a geometrically realistic detonation. The overarching goal of this development effort was to provide a proof of concept to the integration of CFD results into a pattern of life simulation. The accuracy of the CFD results could be refined in future iterations.

Table 3. Comparison of empirical distances to simulation results for the Kalevi Stadium

Peak Overpressure (psi)	Empirical Stand-off distance (ft)	Average Simulation Radius (ft)
0.5	1148	1117
2.0	394	587
10.0	117	230

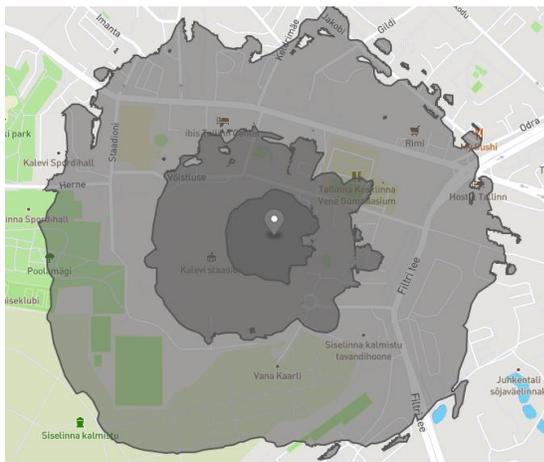


Figure 8. 2D map of the three peak overpressure levels extracted at ground level for the Stadium scenario

In this scenario, most of the stadium is covered by the 2 psi and 10 psi overpressure levels as shown in Figure 8. Multiple injuries and some casualties would be expected amongst the population gathered in the stadium. The detonation doesn't reach the hospital to the west of the stadium (not shown in the figure), therefore limited critical infrastructure would be impacted. This scenario shows a higher impact on the civilian population than the local infrastructure, as opposed to the previous scenario, where multiple buildings would have likely collapsed under the detonation.

CONCLUSION

The integration of high-fidelity blast CFD simulations inside a large-scale pattern of life simulation was presented. Detonations ranging from 5 000 to 10 000 lbs of ANFO in a fertilizer lorry in the areas of Tallinn's Town Square, the Stadium and Freedom Square were simulated. The simulations considered the variability of explosive charge, surrounding infrastructure including buildings, terrain topology and street corridors. The framework was integrated as part of a geospatial digital twin that included detailed urban geography, a large-scale pattern of life simulation, critical infrastructure and 3D visualization and analysis. The blast pressures imported into the digital twin converted spatial and temporal distributions of pressure data into probabilities of human casualties and infrastructure damages. The paper demonstrated the effectiveness of using advanced frameworks and pattern-of-life simulations as a crucial tool for training emergency responders and evaluating the effectiveness of response plans.

The maximum overpressure was computed throughout the simulation of the detonation. This information was then disseminated to the Pattern-of-Life simulation. The results section offers empirical measurements as a comparative solution to the CFD results. Future work could include more complex properties to provide a better representation of such detonations. Properties such as temperature or wind speed could be used to provide more accurate casualty data. Further parameters affecting emergency response time, such as contamination, residual debris or visibility issues could also be added to the simulation. These parameters would be more difficult to determine empirically. Wind speed, for example, is highly dependent on the topography being simulated. As observed with the overpressure radius of effect, the simulation results show an overestimation of the high-pressure area in the detonation simulation. The scenarios studied both used the same explosive type, but a relatively simple detonation method was used to activate the detonation. More analysis is needed to better quantify the effect of more complex detonation methods and explosive charge shape to determine its effect on energy dissipation throughout the detonation.

Overall, the integration of BlastFOAM's multi-fluid CFD solver with a real-time pattern of life simulation showed its potential to improve crisis management training within a safe environment. The large discrepancy between the CFD solver's execution time and the fast refresh rate of the pattern-of-life simulation offers limited on-demand capability at the time of writing and thusly relies on an offline integration of pre-determined scenarios. Future approaches towards scaled cloud infrastructure and more refined CFD algorithms could help bridge the gap between the two simulations.

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