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PHYSICS-BASED EXPLORATION OF EXPLOSION PARAMETER SPACES (PEEPS)

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Final Report

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14. ABSTRACT

We modified the CRAM3D nonlinear finite element code so that it could divide the calculation among processors in two dimensions. We then ran test cases using the updated code and revised the documentation. We also made improvements to the input to make the code easier and more robust to use. After the code modifications were completed and tested, we provided support for users of the code. We delivered the CRAM3D code and documentation to AFRL.

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1. SUMMARY

We modified the CRAM3D nonlinear finite element code so that it could divide the calculation among processors in two dimensions. We then ran test cases using the updated code and revised the documentation. We also made improvements to the input to make the code easier and more robust to use. After the code modifications were completed and tested, we provided support for users of the code. We delivered the CRAM3D code and documentation to AFRL.

2. INTRODUCTION

CRAM3D is a three-dimensional nonlinear finite element code specifically designed for calculations of nuclear explosions. It can handle both 3D topography and multiple nuclear explosions (Stevens and O'Brien, 2018a). CRAM3D uses MPI to split the problem over multiple processors. At the start of this project, MPI could be applied along a single dimension (the X direction). The main objective of this project was to modify CRAM3D to apply MPI along the X and Y directions, which allows it to use many more processors, greatly reducing the time required for each calculation.

3D nonlinear calculations of nuclear explosions are used to develop a physical understanding of the nuclear explosion source and corresponding generation of seismic waves. It addresses the dependence of seismic source generation on small shallow explosion emplacement conditions (depth, scaled depth, decoupling, material properties, pre-stress, and local structure/topography). The changes implemented in CRAM3D allow more complex geometries and emplacement conditions to be calculated.

Understanding of the explosion source is fundamental to nuclear monitoring. In spite of decades of research on this subject, there are still many unknowns, particularly when there is strong topography, tectonic stresses or multiple simultaneous explosions. CRAM3D allows calculations of complex explosion emplacement conditions and can directly address these problems.

CRAM3D can provide insight into the generation of seismic waves that is not possible by any other method. To the best of our knowledge there is no other code that can perform three-dimensional nonlinear calculations of nuclear explosions that include gravity and topography, and then propagate the solution to distant seismic signals.

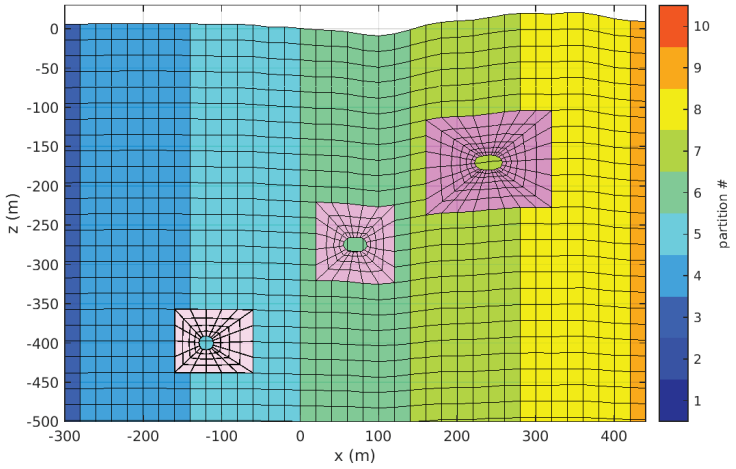

Figure 1 CRAM3D calculates multiple explosions in a structure with gravity and topography. Each explosion is contained in a finely zoned inner grid shaped to match the shock wave from the explosion. CRAM3D divides the outer grid into multiple segments, so that calculation time is inversely proportional to the number of processors. Prior to this project, CRAM3D split the grid only along the X direction. In this project we modified the code to split the calculation in both the X and Y directions, which can reduce calculation time by an order of magnitude or more

We have modified CRAM3D to allow it to use many more processors, greatly reducing the time required for each calculation. We delivered to AFRL an updated version of CRAM3D, together with an updated User Manual and User's Guide. We also provided support to CRAM3D users at AFRL who are using the code.

2.1 The CRAM3D Code

CRAM3D was developed under AFRL support with version 1.0 delivered in 2011 (Stevens et al, 2011a, 2011b) , and it has been continuously improved since then. In 2018, it was modified to allow calculation of multiple nuclear explosions, and a User's Guide (Stevens and O'Brien, 2018b) containing many examples was written and delivered to AFRL to help AFRL and AFTAC personnel use the code. It was recently used in a DTRA project for calculations of 13 underground nuclear explosions at the Degelen Mountain test site (Stevens, O'Brien and Given, 2022) as shown in Figure 2. In that project, a technique was developed to allow a single equilibrium calculation to be performed for the test site (one for the northern section and one for the southern section), after which the inner grid containing the explosion was inserted at the appropriate location in the grid for each calculation with the explosion. Calculations were performed for both topographic and flat surfaces and with and without tectonic stresses, for a total of 39 calculations.

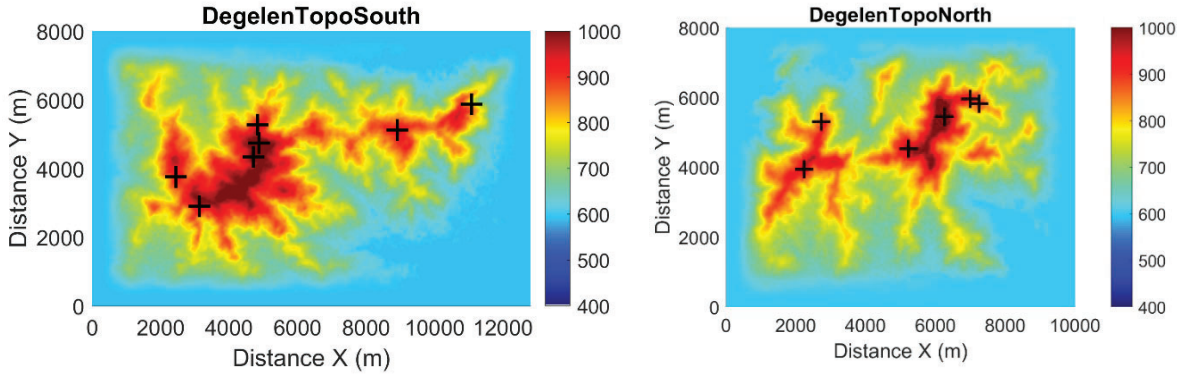

Figure 2 Calculations were performed in the southern (left) and northern (right) sections of the Degelen Mountain nuclear test site. Colors show elevation in meters. Black marks are explosion locations

CRAM3D has also been used for calculations of explosions in North Korea (Stevens and O'Brien, 2018c), Novaya Zemlya (Stevens, O'Brien and Given, 2022) and the Rainier Mesa and Pahute Mesa areas of the former Nevada Test Site (Stevens and O'Brien, 2023).

CRAM3D has been developed over more than a decade and used to solve a number of large problems, so the technology is quite mature. The history of the code is actually much longer, as it was derived from an earlier axisymmetric code CRAM that was developed during the nuclear containment program (e.g. Nilson, Rimer and Halda, 1991). Although the structure of CRAM3D is more modern and quite different, CRAM3D includes material models from CRAM that were developed over many years based on nuclear explosion data.

3. TECHNICAL APPROACH

3.1 Modification of CRAM3D to support MPI partitions in two dimensions.

CRAM3D is written entirely in Fortran 90, with some Fortran 95 and Fortran 2003 extensions, and uses MPI (Message Passing Interface) to split the calculation among multiple processors. CRAM3D was implemented and tested using MPICH2[1].

Following is an outline of the computational scheme used by CRAM3D:

1. Input to the calculations is read by subroutine *gen*, and the grid is generated in subroutine *meshfem3D*. Both the inner and outer grids are generated, and the grid is split into regions to be managed by each processor under MPI. Material properties are assigned to grid blocks and overburden pressure due to gravity is placed in the grid.
2. Subroutine *cramfem3D* drives the code through each cycle until the input stop time or stop cycle number is reached. On each cycle, cramfem3D calculates the cavity pressure, rezones the inner grid if requested, calls the main computational routine *calca*, then outputs results at times specified by input.
3. Subroutine *calca* calls *zone*, which is the main routine for zone-centered calculations. Zone calculates pressures using an equation of state and deviatoric stresses using Hooke's law with input elastic moduli. Deviatoric stresses are compared with a strength model and adjusted when strength is exceeded. *Calca* then calculates effective forces at each node, calculates acceleration and updates velocity and displacement at each node.

Each processor calculates all of the quantities internal to the regions that are managed by that processor. At the end of each cycle, each processor uses MPI to exchange information on the boundaries between neighboring regions and then sums the calculated forces on each boundary so that the net result is identical to running the calculation in a single grid.

Using MPI requires a lot of bookkeeping to ensure that the necessary information is exchanged across all boundaries. Prior to this project CRAM3D used one processor for each inner grid and divided the outer grid into parallel regions in the X direction (see Figure 1, for example). Each region can have a thickness as few as two zones, and the increase in speed is approximately equal to the number of processors used. To use additional processors in the Y direction we need to ensure that information is transferred correctly across all X and Y boundaries in the outer grid and between outer grids and the inner grid(s). Doing this correctly for the inner grids is complicated because they may intersect several outer grid regions.

3.2 Test Cases

The test cases in the User Manual and examples in the User's Guide exercise almost every option in CRAM3D, so we used these as test cases for the modified code. When correctly implemented, the results are independent of the number of processors in both the X and Y directions. In the following, we describe these test cases.

[1] MPICH2 is available for download from http://www.mpich.org/.

3.2.1 User Manual Test Cases

The User Manual (Stevens and O'Brien, 2022a) has included an example test case since the first version of CRAM3D. It is a calculation of a 5 kiloton explosion at a depth of 402 meters in Degelen Granite with a prefractured layer above and a weak material on one side of the explosion (Figure 3). This geometry generates SH waves due to the asymmetry caused by the weak region.

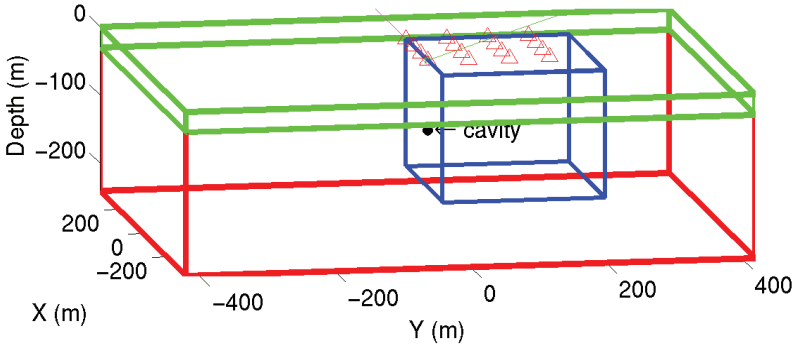

Figure 3 Test calculation #1: 5 kiloton explosion in granite next to a weak inclusion. Only the central part of the grid is shown; the full grid extends to ±700 meters in the X and Y direction and to 780 meters depth. The cavity center is at 402 meters depth, deeper than shown in this illustration

The second test case in the User manual is a calculation of the NPE named "NPE-20m." The NPE-20m test case is modeled after the NPE calculation (Stevens, Thompson and O'Brien, 2014), but with a larger grid spacing so that it can run in a short time (<1 hour). It contains three subcases – topo (with topography), notopo (without topography), and topo_tapered, with topography tapered to be flat outside the monitoring surface (Figure 4).

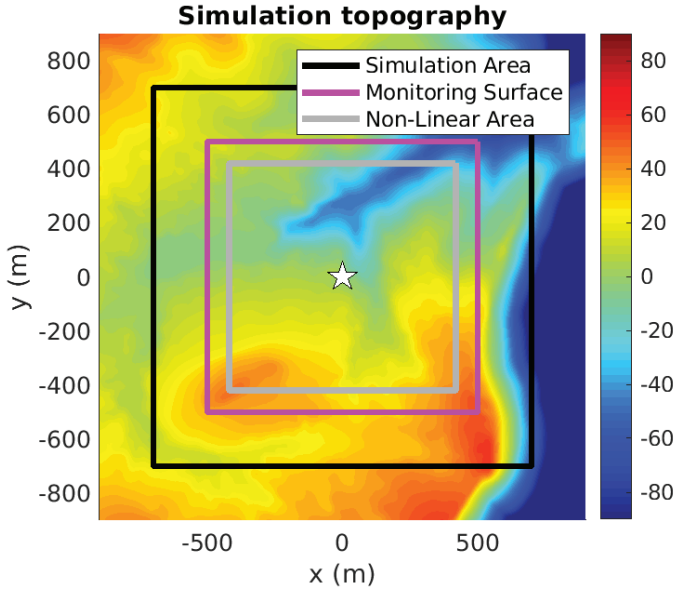

Figure 4. Test calculation #2: NPE. The surface is tapered to a common elevation at all points outside the Monitoring Surface

3.2.2 User's Guide Test Cases

The Cram3D User's Guide (Stevens and O'Brien, 2022b) is intended to introduce new users to all of the capabilities of CRAM3D as a starting point for performing new calculations. It therefore provides an excellent set of test cases for testing the modified code. It contains the following examples:

1. Shoal: Rectangular grid with a granite material model and an explosion with a 12.5 kiloton yield (corresponding to the explosion Shoal).
2. Shoal with prestress: Shoal model with tectonic prestress added published in Stevens and Thompson (2015).
3. Topography: A simple topography model, adding a mountain on top of the Shoal model (Figure 5).
4. Cavity decoupling: Detonating a much smaller 0.1 kt explosion within the Shoal cavity.
5. North Korea: A much more complicated case, four explosions at different depths in the actual topography of the North Korean nuclear test site (Stevens, O'Brien and Thompson, 2017).
6. The Non-Proliferation Experiment (NPE): this is the full resolution calculation of the NPE discussed in the previous section.
7. Multiple Explosions: Simulation of the Soviet explosion Dnepr2 (Stevens and O'Brien, 2018a), two 1.7 kt explosions separated by a distance of 75 meters at a depth of 175m (Figure 6).
8. Micromechanical Damage Model: the Shoal explosion modified to include the micromechanical damage model developed by Prof. Charles Sammis (Stevens, Sammis and O'Brien, 2021).

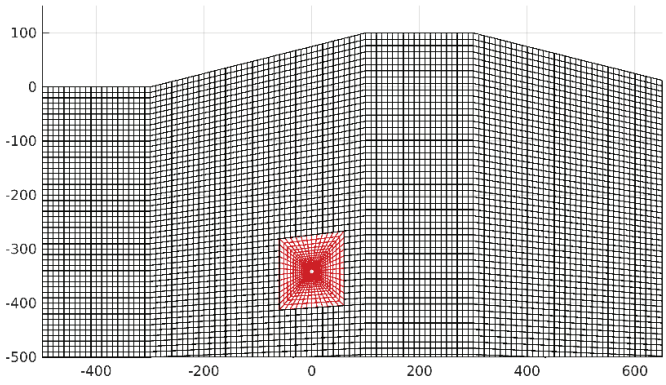

Figure 5 Grid for the simple topography model. The inner grid is shown in red

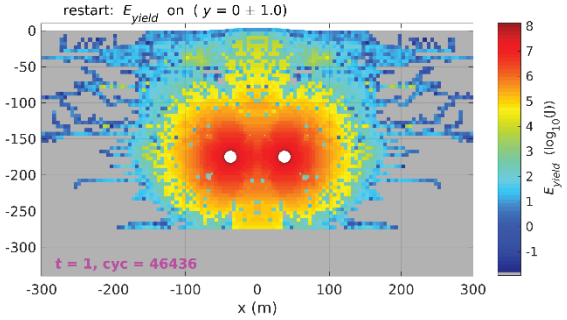

Figure 6. Final plastic work in Dnepr2 calculation of a double explosion

4. RESULTS AND DISCUSSION

We delivered the code, documentation and test cases in October 2022. We presented the results of this project at the AFRL TIM on January 31, 2023 (O'Brien and Stevens, 2023). After that time, we provided support for AFRL personnel using the code, responding to questions as needed.

4.1 What Factors Control Run Time?

The run time is controlled by several factors. MPI runs a calculation for each inner grid and each outer grid partition in a separate processor, but the run time will be controlled by the slowest partition as the calculation will wait until all processors have finished a time step. The controlling factors are:

1. Size of the outer grid – a large grid will have $O(10^8)$ zones in the outer grid.
2. Size of the inner grid(s) – large inner grids typically have $O(10^4)$ zones.
3. Number of processors over which the calculation is split.
4. Time step – controlled by the smallest zone size in the grid, almost always in the inner grid. Rezones in the inner grid(s) are essential to increase the time step once the shock wave has passed.
5. MPI data exchange volume - adjacent processors exchange data after each time step.
6. Disk IO - CRAM3D processors potentially write many large grid files.

The relative importance of these factors is summarized in the Table 1. As an example, suppose the grid is 100x100x80 zones. With 1-D partitioning, the maximum number of processors that can be used is 50. With 2-D partitioning, the maximum number of processors that can be used is 2500, and in 3D 100,000, so there is a potential huge gain in increasing the dimensionality. With 3D partitioning, however, the inner grids may have more zones than the outer grid partitions, in which case the inner grids control the run time, so much less is gained by adding the third dimension than the second.

Table 1. Run time dependence for partitions in one, two and three dimensions

Dim	Max # Procs	Min # Zones /Proc	MPI Exchange Nodes for M Procs
1-D	$N/2$	$2N^2$	N^2M
2-D	$N^2/4$	$4N$	$2N^2M^{1/2}$
3-D	$N^3/8$	8	$3N^2M^{1/3}$

4.2 Performance Test Case

As a test case to assess the performance difference between 1D and 2D partitioning, we compare two calculations of Novaya Zemlya explosion B-1 partitioned in one and two dimensions, respectively. This test had four separate explosions as shown in Figure 7 and Figure 8, with a total yield of 3.8 Megatons, slightly less than the 4.2 Megatons shown on Figure 7. The calculation is described in detail in Stevens et al (2022).

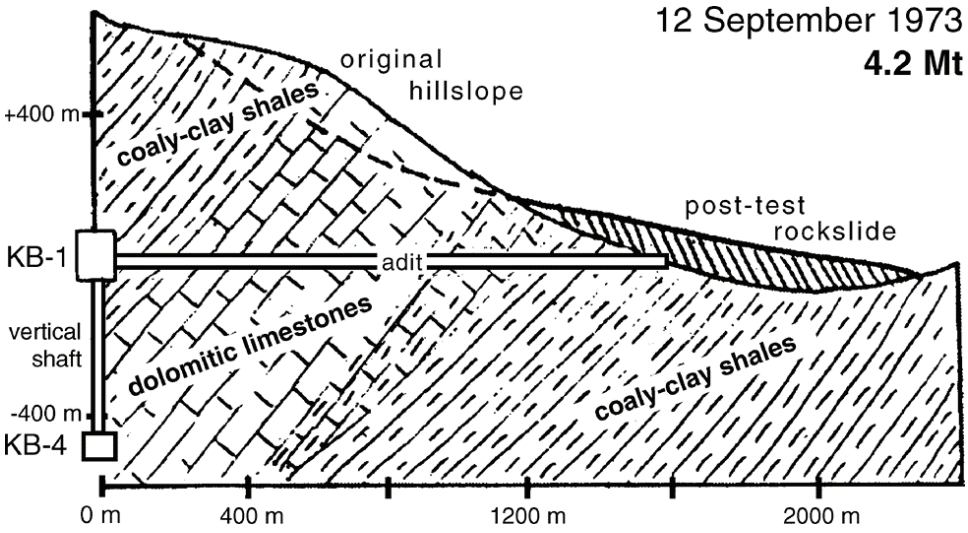

Figure 7. Slice through the center of the B-1 test. KB-4 was the deepest and largest explosions (2.6 Megatons), while there were three explosions of 400 Kilotons at the depth shown for KB-1. The figure is from Khalturin et al (2016)

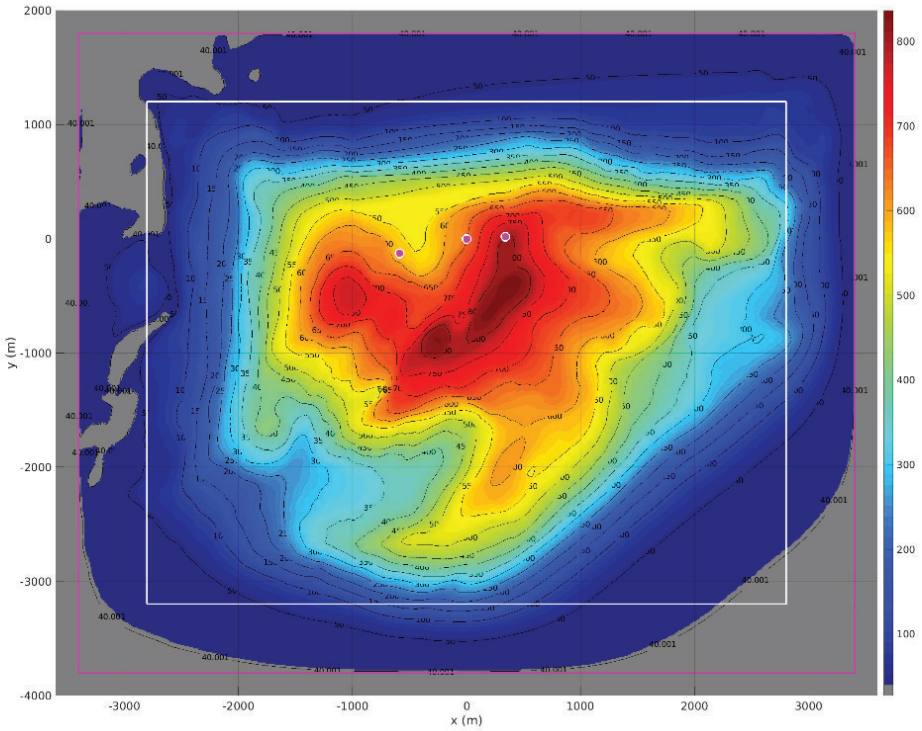

Figure 8. Topography near Novaya Zemlya explosion B-1 with three horizontal locations marked

We ran one calculation of Novaya Zemlya explosion B-1 partitioned along the X direction with 179 processors, and a second calculation partitioned along the X and Y directions with 1004 processors. This test had four explosions, so in both cases four processors were used for the inner grids. 2D partitioning divided the outer grid into 50x20 partitions. The grid dimension was 350x300x90 for 1D partitioning and 350x300x140 for 2D partitioning and both calculations were run to 10 seconds. The second calculation was extended to a deeper depth because the nonlinear deformation extended quite deep for this large test (Figure 9) and the first calculation cut off some of this nonlinear region.

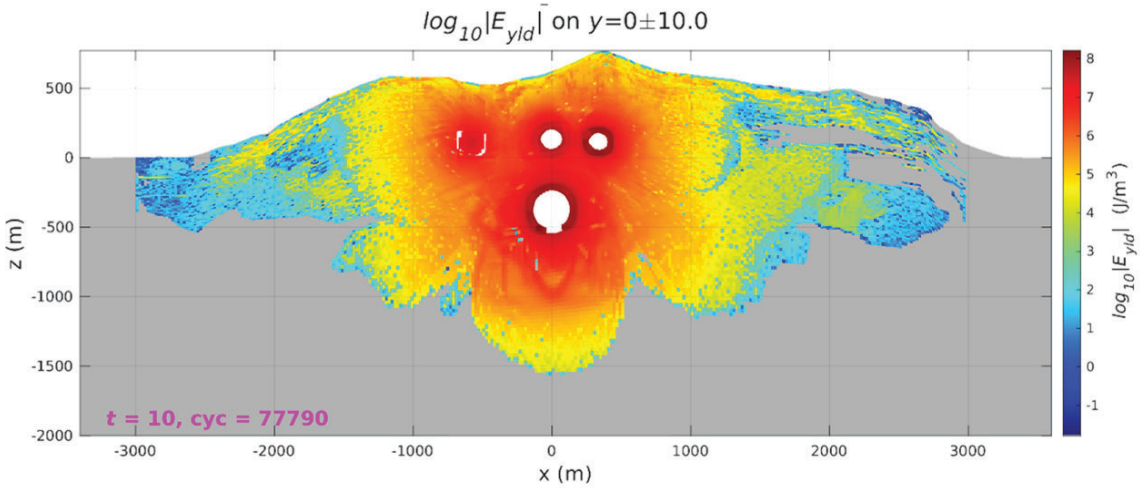

Figure 9. Nonlinear deformation (plastic work) at the end of the Novaya Zemlya B-1 calculation

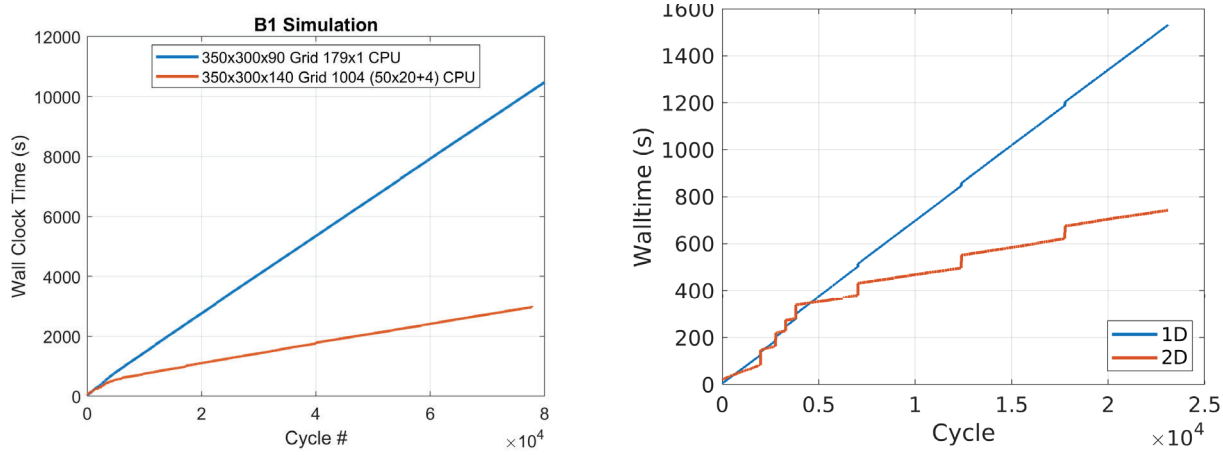

Figure 10. Left: wall clock time for calculations partitioned in one dimension (blue) and two dimensions (red). Right: expanded view of the earlier part of the calculations showing I/O jumps

Figure 10 shows the wall clock time for the two calculations. The slopes indicate that 2-D-partitioned simulation consistently advances about 3.7X faster than 1-D as expected. There is also no evidence that MPI data exchange is rate limiting. As shown in the right panel there are jumps in time whenever the grids are written, indicating that I/O is slower with more processors. The reasons for this are not clear, but this is a minor issue for a long calculation.

4.3 Calculation Times

The following times are from calculations on an HPE SGI 8600 system (Mustang).

Table 2. User's Guide Calculation Wall Clock Times

Calculation	# CPUs	nprocx	nprocy	Equilibrium Run Time (Minutes)[2]	Explosion Calc Time (Minutes)
Shoal	1001	100	10	1.35	14.86
Decouple	1001	100	10		20.60
SimpleTopo	1001	100	10	3.95	14.55
Prestress	1001	100	10	1.87	12.48
MicroDamage	1001	100	10	1.63	14.48
NPE	1015	78	13	14.78	78.43
Dnepr2	1002	100	10	2.00	26.48
NK	1001	100	10	31.77	25.66[3]
Degelen[4]	1015	78	13	3.23	32.9

Table 3. User's Guide Calculation Parameters

Calculation	nx	ny	nz	Equilibrium End Time (Seconds)	Explosion End Time (Seconds)
Shoal	200	200	80	0.5	3.0
Decouple	200	200	80		0.5
SimpleTopo	200	200	80	10.0	3.0
Prestress	200	200	80	2.0	3.0
MicroDamage	200	200	80	0.5	3.0
NPE	234	234	140	20.0	3.0
Dnepr2	200	200	80	0.5	1.0
NK	400	340	140	25.0	3.0
Degelen	234	234	130	1.0	2.0

[2] All equilibrium runs were used the "noinner" parameter. Decouple used the equilibrium run from Shoal.
[3] Average of calculations at four depths. Individual calcs range from 23.38 to 27.38 minutes.
[4] Degelen is the example in the User Manual. Input files are now included with the User's Guide input files.

4.4 Input improvements

In addition to the performance improvements discussed in the previous sections, we also modified the input to the code to make it easier to use and more robust against erroneous input. In the early versions of CRAM3D, all input was specified in a fixed format file that required all input parameters to be entered in a specified order. Most of the input can now be defined through parameters, which can be input in any order, and can be separated into multiple files. The fixed format file now contains only material property and source and grid information. All other inputs are parameters, which can be included in the fixed format file or separated.

The recommended approach is to include in the fixed format file all parameters that are the same in both the equilibrium run and simulation run, but separate out the inputs that are unique to each run. Details of the parameterized input are given in section 2 of the User Manual (Stevens and O'Brien, 2022a). The User's Guide (Stevens and O'Brien, 2022b) contains examples for all of the cases described above in section 3.2.2.

5. CONCLUSIONS

We have modified the CRAM3D code to make it capable of performing much larger calculations in a much shorter time. This was accomplished by dividing the grid into partitions in two dimensions instead of one, which allows many more processors to be used in the calculation. This allows more calculations to be done in a shorter time, thus allowing "exploration of explosion parameter spaces." In addition, we modified the input to the code to make it easier to use and more robust by parameterizing much of the input.

All of the examples in the User's Guide were modified to optimally use the new input parameters and to be partitioned in two dimensions. All of the examples in the User's Guide and the User Manual were run and compared with prior results to test the revised code and to ensure consistency of results.

The code, User's Guide and User Manual were delivered to AFRL, and we have provided support to AFRL personnel in the year since code delivery.

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List of Symbols, Abbreviations, and Acronyms

AFRL	Air Force Research Laboratory
NTS	Nevada Test Site
PEEPS	Physics-based Exploration of Explosion Parameter Spaces
USC	University of Southern California

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