# GEANT4-based simulation of a micro-CT scanner using cloud resources

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Research of methods of material recognition using Medipix-based micro-CT scanner MARS requires detailed simulation of passage of X-rays through the sample. The application based on the Geant4 toolkit has been developed to solve this task. Since the computation turned out to be very time consuming for a single PC (several hunderds of projections must be simulated for each sample) the cloud resources has been used. Amazon was chosen as an organization to provide us with such a resources and, particularly, its cloud computing related service - AWS (Amazon Web Services). Two possible ways to create the AMI (Amazon Machine Image) with installed software for the problem was considered. This AMI was used to run instances (virtual server) to perform calculations. A significant increase in performance was reached by using several instances that were working at the same time (the task can be divided into independent pieces). A job submission framework optimized to run Geant4 applications in Amazon EC2 has been implemented using Python language. All actions after registration on AWS (Amazon Web Services - cloud computing service) to run instance - virtual server - are explained. We considered 2 ways of AMI creation (Amazon Machine Image - template of the instance). The first way is to use template given by Amazon and install any required software on it. The second way is to create template using one of prepared virtual machines with some preinstalled software. We used this template to create a lot of instance that worked at the same time computing different parts of the calculation. Use of this method lowered time of computation and made it acceptable. Obtained results were compared with expectations, we consider our method to be effective for our task.

Keywords: cloud computing, circular cone-beam CT, GEANT4, Python, Amazon Web Services, Medipix

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# Introduction

Our group studied problem of material's chemical composition recognition using CT scanner MARS(Medipix All resolution System) – the first commercially available 3D spectral (multi-energy) scanner to produce images with anatomic and molecular quantification at a fraction of the cost, time, and radiation dose of traditional molecular imaging, such as PET or SPECT. It is based on Medipix detector chip [Ballabriga, Campbell, ..., 2011] - CMOS pixel detector readout chip designed to be connected to a segmented semiconductor sensor, developed by the Medipix3 Collaboration.

This task requires simulation of the CT scan to improve accuracy. Elements can be recognized using only their mass attenuation coefficients and its dependency on energy of X-ray but it leads to large errors. Computer model helps to take into account features of the sample, geometrical defects, beam hardening. Our program imitates the real scan of the multi-contrast phantom for material decomposition, calibration and quality assurance. It is written in C++ language and uses the Geant4 toolkit [Allison, et al., 2006] for simulation of passage of X-rays through the samples.

Monte-Carlo simulation requires a lot of computing power to simulate a large number of radiation quanta and their interactions with matter. This led us to the idea of using cloud-computing resources. We chose an organization to provide us with such resources – Amazon [Ostermann, Iosup, ..., 2010]. In particular, cloud computing related service of Amazon is called AWS (Amazon Web Services). Amazon EC2 (Elastic Cloud) forms the central part of it. To perform this work we also need the storage service - Amazon S3 (Simple Storage Service). Amazon EC2 provides us with a so-called instances - virtual servers with certain operating systems. An instance type is determined by this system and the resources assigned to it. The cost of the instance (per hour) is defined by resources. Instance considered to be running, even if it is not performing any useful work.

# Application

Our computer program simulates the real CT-scan. The simulated setup consists of X-ray source, studied sample and detector. X-ray source generates gamma quanta which momentum is distributed evenly in a cone. Energy of quanta is distributed according to the real X-ray tube spectrum:

As samples, we created 2 different objects for different kinds of experiments. First sample is cylinder containing several small cylinders inside. This object was used to study material recognition and simulates syringes with fluids in a stand. Second sample is a rectangle with circular grooves and stripes. It is used to determine the size of smallest details that scan is able to register. Particular interest has the dependency of this size on geometrical defects of the setup.

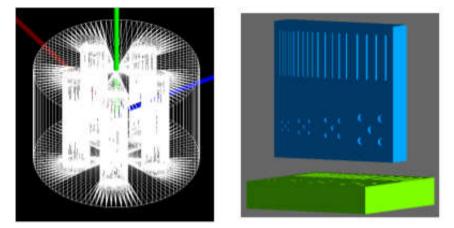


Fig. 1. Simulated samples

During the simulation gamma quanta are generated in focal spot of X-ray tube and pass through the phantom. They are registered on the detector at different energy thresholds. This procedure is applied for 360 angles with step of 1°. CT reconstruction programs use this data to recreate a sample [Turbell, 2001]. Reconstruction algorithms are based on the equation which determines the intensity of the beam passing through matter:

$$I_{out} = I_0 e^{-\int f(\vec{r})dl} \tag{1}$$

These algorithms determine f(r) – effective mass attenuation coefficient of different points of sample and this allows to recognize the material. The main feature of MARS is the ability to measure the intensity of quanta with energies above the thresholds (8 thresholds can be set at the same time). This allows to measure the dependency of mass attenuation coefficient on energy and greatly improve the accuracy of recognition.

Our computer model is able to simulate different defects of the experimental setup such as focal spot nonzero size, X-ray tube displacement and rotation axis displacement. These problems affect the quality of the reconstructed volume. Usually they lower contrast of the output images and reduce the visibility of details. Rectangular sample with grooves and stripes was used to study these effects.

#### Calculations

SSH client is used to connect to instances so it has to be installed on the client machine. To use Amazon EC2 services one should perform several steps to provide convenient and safe access to his resources. Firstly, one has to sign up for AWS, after that it is desirable to create an IAM (Identity and Access Management) user to restrict users credentials and add this user to created administrators group. AWS also uses public-key cryptography to secure the login information for the instance, so one should (in case of Linux instances has to) create key pair. For security reasons one should create security groups for for instances to restrict range of IP, from which one can get access to the instance.

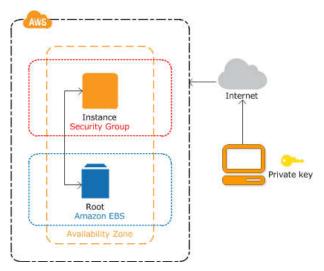


Fig. 2. Connection to an instance

One can only create an instance using a certain template, called AMI (Amazon Machine Image). There are two basic ways to create an instance: one may use a standard template provided by Amazon, or create his own template by using a user's operating system. The main advantage of the first method is that there is no need to configure and load his own operating system, one can instead use one of the

relatively wide range offered – among these templates are Amazon Linux AMI, Red Hat Enterprise Linux, SUSE Linux Enterprise Server, Ubuntu Server, a lot of Windows servers, etc with different initial settings. Among the shortcomings - there is a need to configure the system that is already in progress and load tools for a specific task directly in the instance. Moreover, these operations are not always possible due to the limited number of standard AMI. However, a customized system can be saved as a template and can be used to create a number of instances, which is very useful if the task can be divided into independent pieces and one configuration is suitable for each of them.

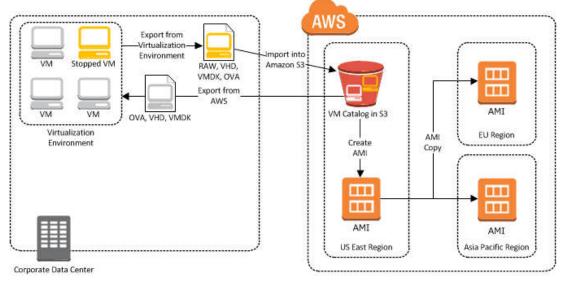


Fig. 3. Creation of an AMI

The second method is more suitable if the specific properties of specific operating systems are required for solving the problem, as well as if an environment for Computing System was created a long time ago and it is difficult to completely transfer all necessary components to a clean operating system. Disadvantages include a comparative inconvenience (compared with the first method) of the procedure of creating an instance (especially for simple tasks) which is because one has to perform a lot of additional actions to make it possible to Amazon services to transform loaded virtual machine into AMI. Another point is the requirement to raise additional service - Amazon S3 - service for data storage. One have to connect to an instance via ssh so it has to be installed in the virtual machine before its transformation into the proper format to be loaded into Amazon S3. A full list of essential preparations and acceptable operating systems is contained in the Amazon EC2 documentation pages. Standard templates already have ssh server. There is the other essential tool to be installed on the client – AWS CLI (Command Line Interface), which is essential when one loads VM into S3. CLI is also may be useful for setting properties of AMI users, security groups, etc.

During the work we could install the necessary software (the main component of which is Geant4) on an instance, created on a standard template provided by Amazon, and on the virtual machine OS: Debian 64bit. After that we exported the VM from its virtualization environment and, imported it to Amazon S3 bucket and, in the end, imported it as an image to Amazon EC2, so it was ready to use.

We used Python script for all calculations. Module boto3 helped us to control instances and module Paramiko was used to provide ssh protocol. Overall script creates necessary amount of concrete type of instances, then calculates, processes errors, deletes instances and finally shows us the result.

# Results

A substantial increase in performance over a PC was achieved by running instance 361 for data reduction for each degree separately. PC Configuration: Intel Core i7-3610QM @ 2.30GHz. Configuration of instance on Amazon: Inter (R) Xeon (R) CPU E5-2676 v3 @ 2.40GHz. 10^7 particles on the PC: 3 minutes on Amazon Instance: 2 minutes. 8.5^10 particles per Instance are counted for 40.8 hours. At the same time, it has been used the least productive of the supplied hardware configurations, as the only significant feature was the performance of the processor, and also due to the fact that the version Geant4, does not support parallel execution on multicore processors. Tests have also shown that switching on more expensive instances doesn't affect performance considerably. Namely, 0.5 Gb RAM is enough to perform all the calculations (but is not enough to install all the components on a running instance) and increase in this value doesn't affect this situation.

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