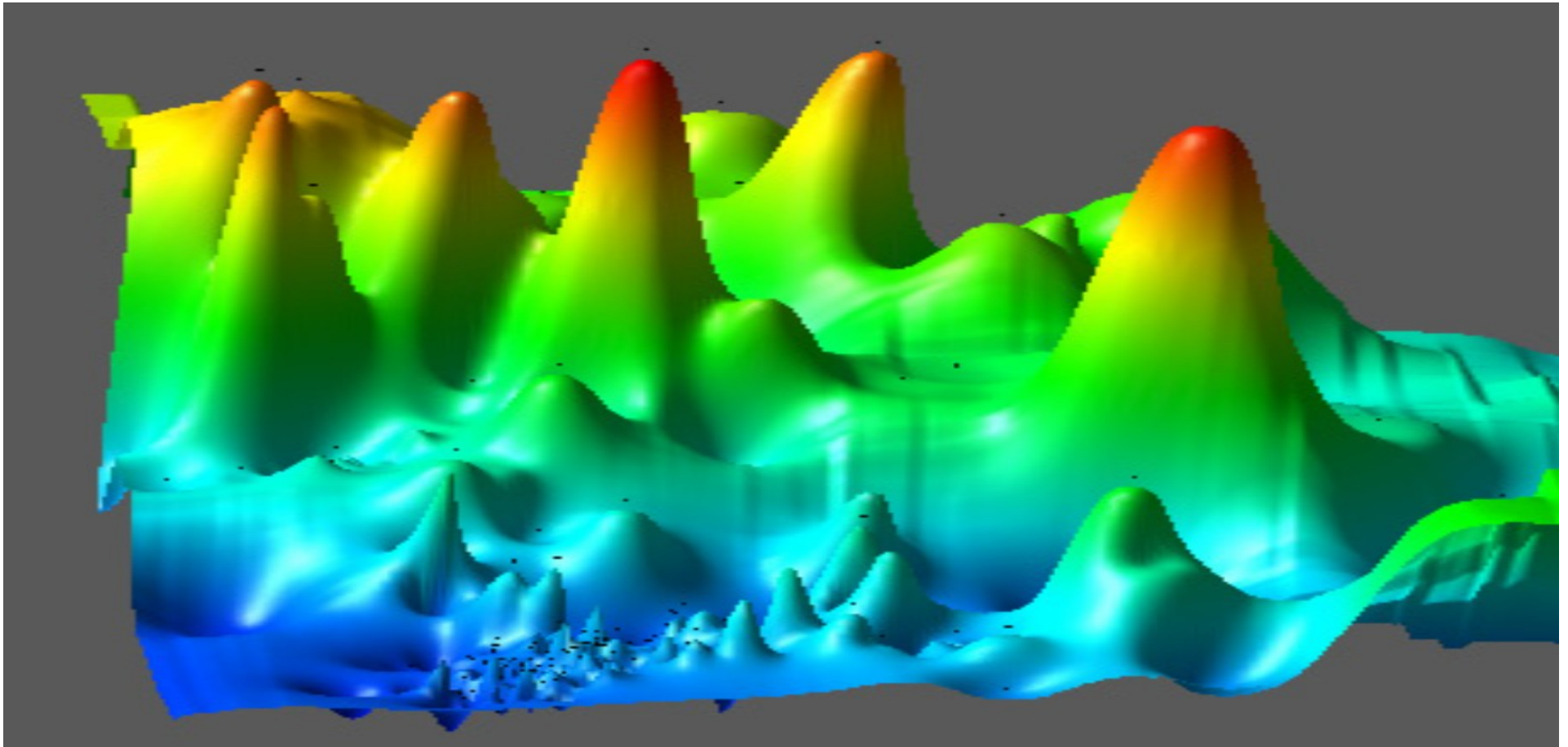# Using Virtualization Technology within Volunteer Computing for Computational Material Design
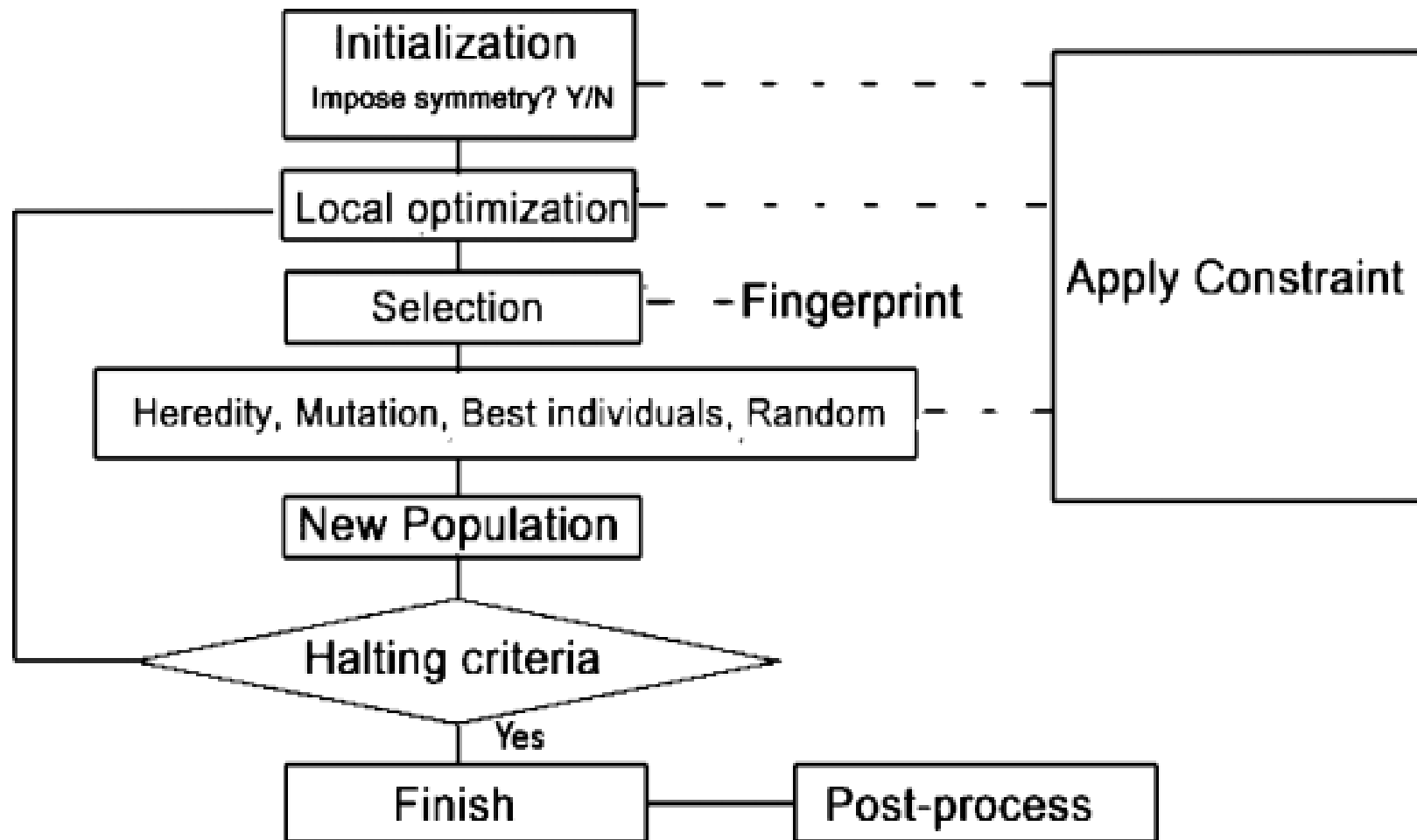
Authors: Nikolay Khrapov, Artem Oganov, Mikhail Posypkin, Valery Roizen, Artem Samtsevich and Vladimir Sukhomlin

Computational materials design

2D-representation of the energy landscape of Au_8Pd_4.

Evolutionary algorithm
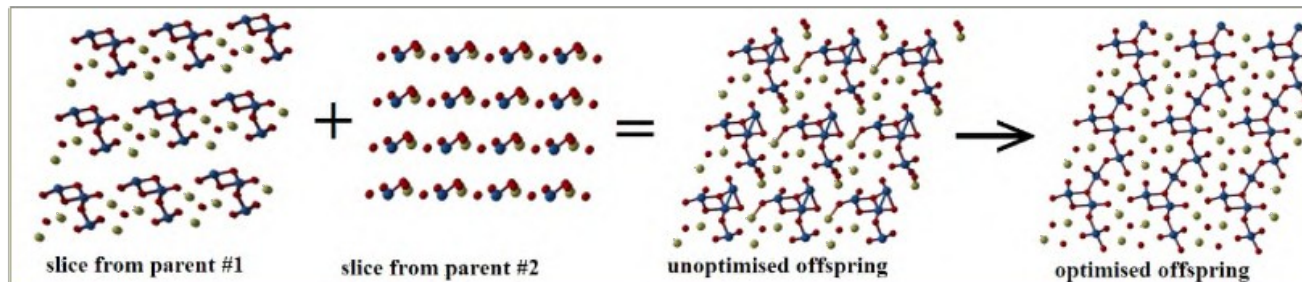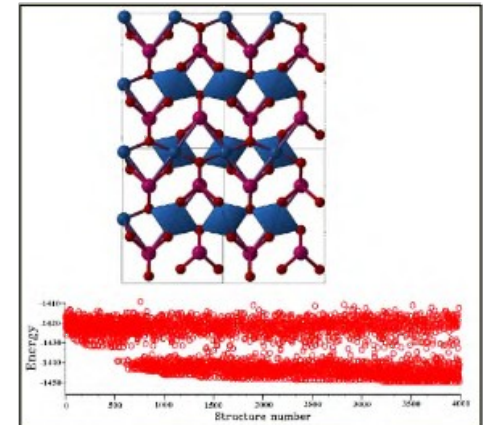
Universal Structure Predictor (USPEX)

Technical features:

- USPEX is interfaced with many ab-initio codes, such as **VASP**, SIESTA, **GULP**, Quantum Espresso, CP2K, CASTEP, LAMMPS, and so on.

- USPEX is devepoled using Matlab;

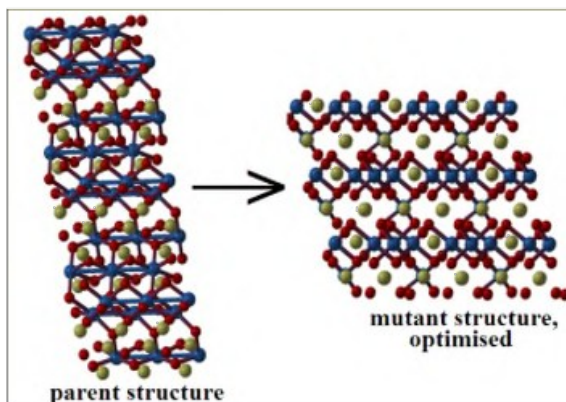- USPEX is compatible with UNIX-like operation systems only.

USPEX
(Universal Structure Predictor: Evolutionary Xtallography)

- (Random) initial population
- Evaluate structures by relaxed (free) energy
- Select lowest-energy structures as parents for new generation
- Standard variation operators:

slice from parent #1   +   slice from parent #2   =   unoptimised offspring   →   optimised offspring

(1) Heredity (crossover)

parent structure → mutant structure, optimised

(2) Lattice mutation

parent structure → permutated structure
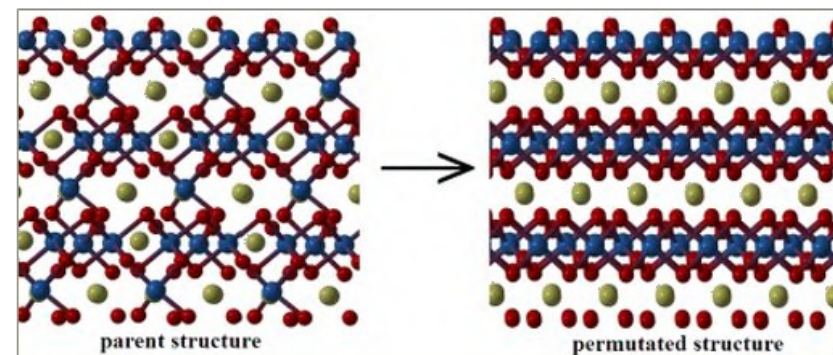
(3) Permutation

Software for local optimization

- General Utility Lattice Programm (GULP)

- Vienna Ab-initio Simulation Package (VASP)

General Utility Lattice Program (GULP)

Features:

- GULP uses classical mechanics;

- GPL; data is not a subject of intellectual property;

- There are versions for Windows, Linux and Mac OS.

- The required computing resource is not huge.

Vienna Ab initio Simulation Package (VASP)

Features:

- There is version only for Unix-like operation system;

- Special license;

- POTCAR is a subject of intellectual property.

- VASP Requires large computational resources;

Approaches

- Launch executable on the volunteer's nodes;

- VirtualBox wrapper;

- Special wrapper.

New approach

- The VM starts on the volunteer's computer from the saved state. Thus, application contains a paused virtual machine.

- The virtual hard disk image contains an encrypted partition. VASP executable is located in this partition.

- The VASP data files are located inside the encrypted zip-archive. The zip archive is located on the portable vdi-image that is stored inside BOINC workunits.

VirtualBox Teleporting

- Starting with version 3.1, VirtualBox supports "teleporting" -- that is, moving a virtual machine over a network from one VirtualBox host to another, while the virtual machine is running. This works regardless of the host operating system that is running on the hosts: you can teleport virtual machines between Solaris and Mac hosts, for example.

VirtualBox controlvm

- Controlvm is other feature of VirtualBox. It is similar as teleporting.

- Preparing VirtualBox image:
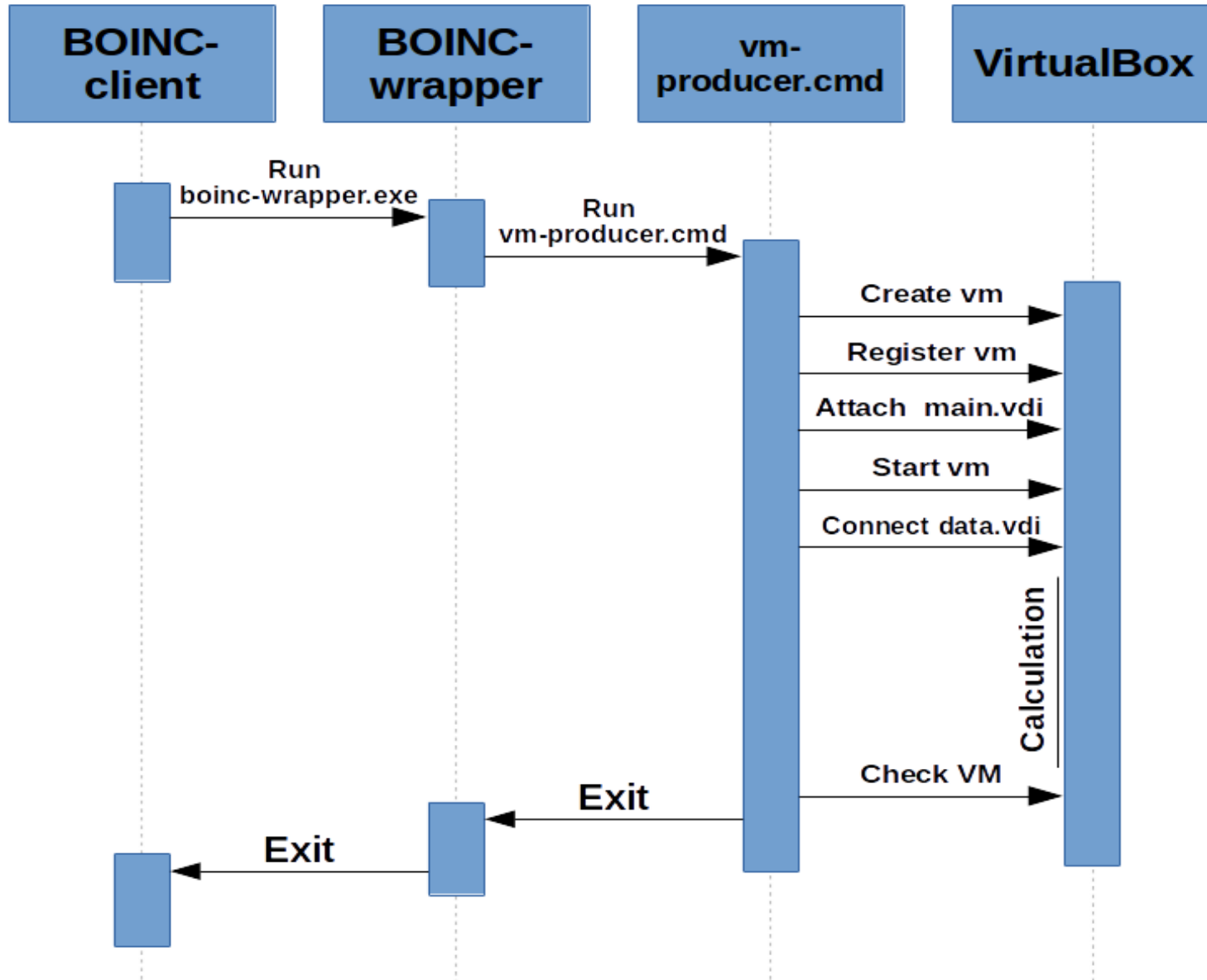
  virtualbox controlvm savestate

- On the client side:

  virtualbox controlvm adoptstate

  virtualbox startvm

Application version

- vdi-disk with the Linux OS and the encrypted partition;

- sav-snapshot of the virtual machine;

- vm-producer.cmd control script;

- BOINC-wrapper and job.xml for it.

Application

Vasp-producer.sh

Running VASP is managed by the vasp-producer.sh script which takes the following actions:

- waits until data.vdi is registered as an external SATA hard drive ("datadrive" in the sequel);

- mounts the data-drive;

- copies zip-file with VASP input files from data-drive to the encrypted disk;

- decrypts zip-file;

- launches the VASP application;

- encrypts results and copies them to the data-drive;

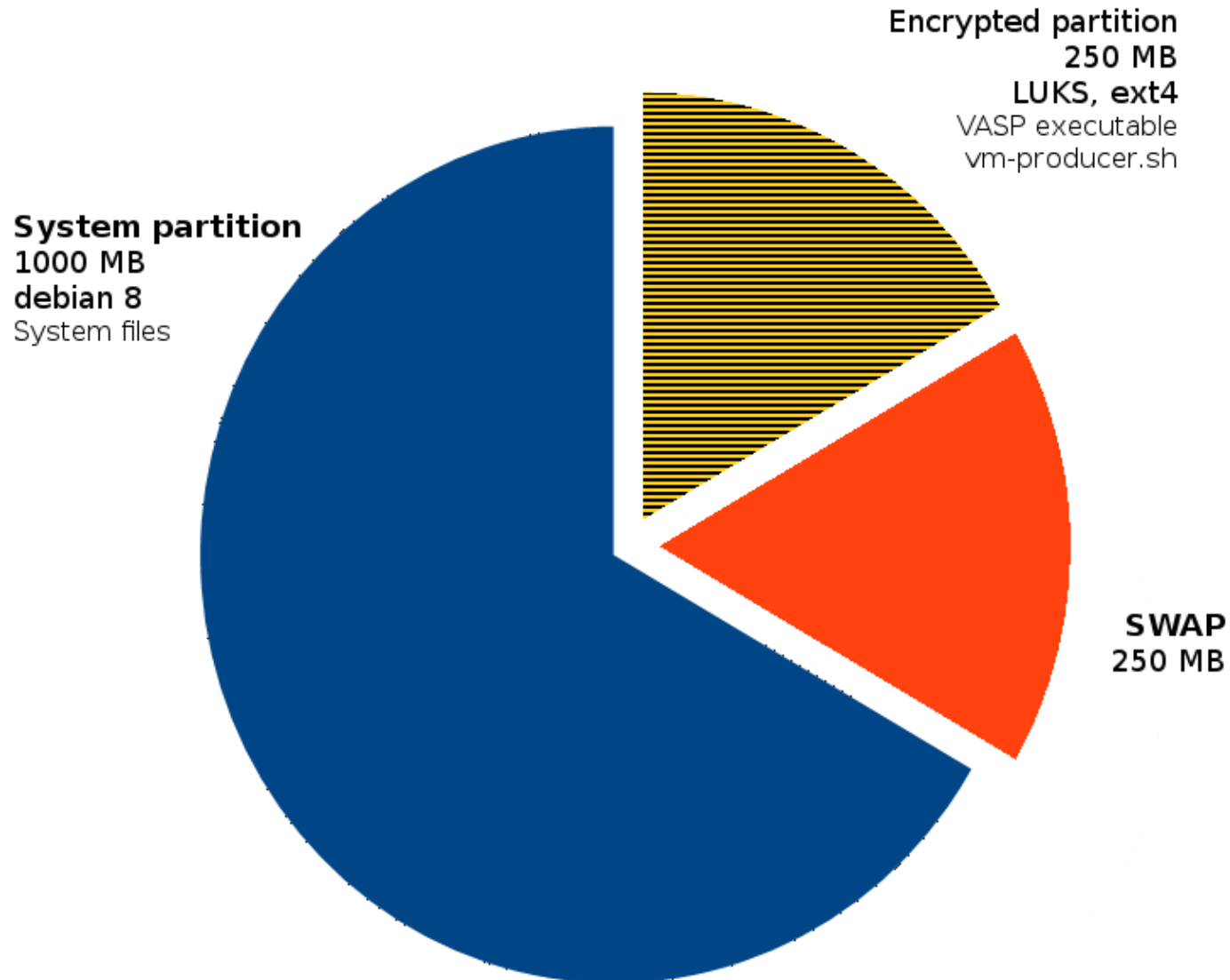- vasp-producer.sh shutdowns the operating system after VASP has done.

Infrastructure
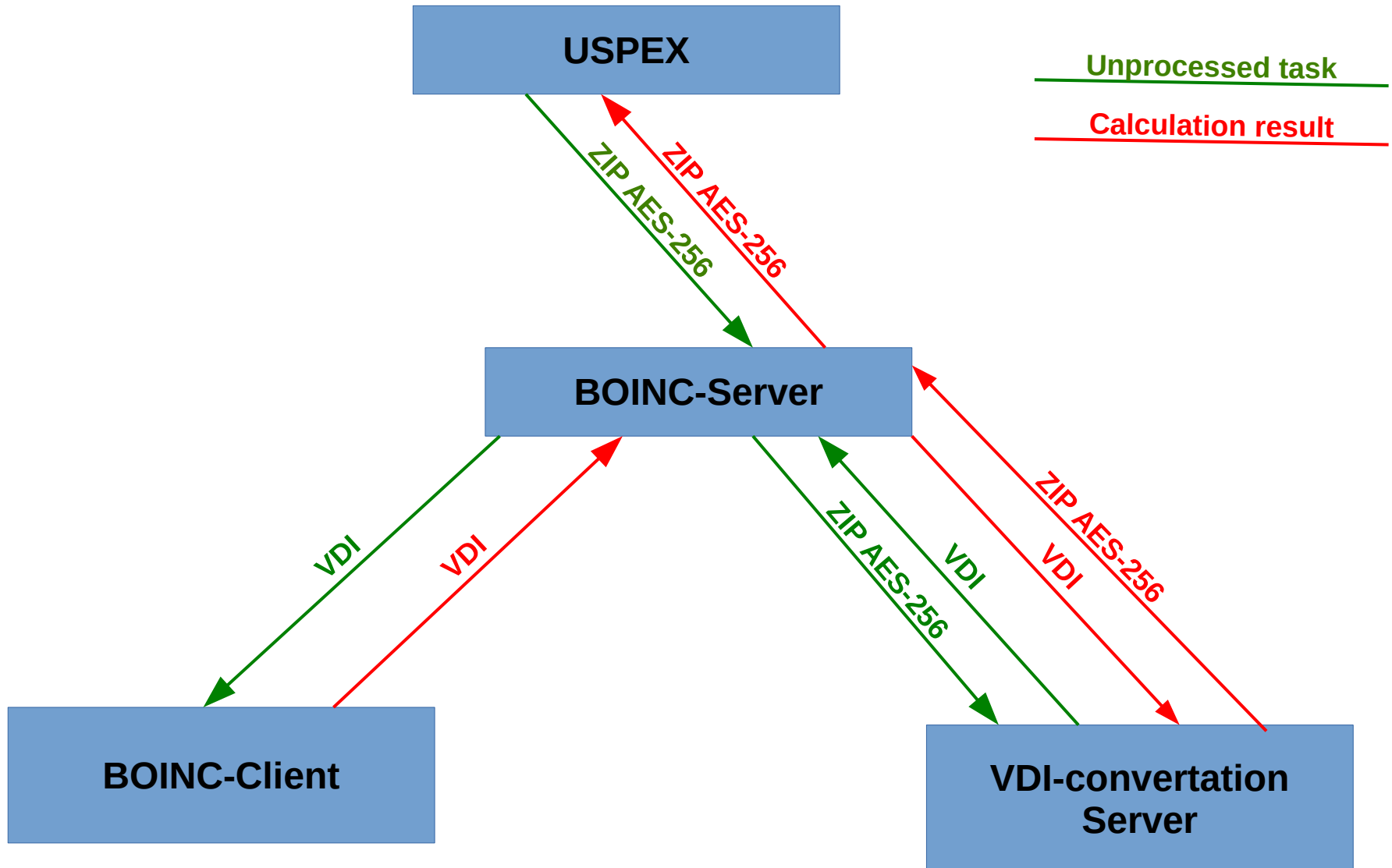
Sizes

Type	Initial	Compressed
Virtual machine VDI	1500MB	300MB
VASP data	≈1MB	15KB
Data VDI	15MB	20KB

Virtual hard disk

Encrypted partition
250 MB
LUKS, ext4
VASP executable
vm-producer.sh

System partition
1000 MB
debian 8
System files

SWAP
250 MB

Conclusion

- We proposed a new universal approach to use proprietary software in a volunteer computing framework. The approach is based on the VirtualBox virtualization technology. The protection is provided by using encrypted folders and password protected archives. This approach was successfully applied in USPEX@home project aimed at computational materials discovery.