

Enclosure 1b. Category 1 Application form 2015 – English version

APPLICATIONS ARE PREFERABLY DRAWN UP IN ENGLISH. AN ENGLISH TRANSLATION HAS TO BE ENCLOSED WITH APPLICATIONS SUBMITTED IN DUTCH.

The application form is available in Dutch on the website <https://vscentrum.be/>.

Title of the application:

Ab initio prediction of acoustic anisotropy of Fe, Ni, and FeNi in the Earth's inner core

Name and first name of the applicant:

Jaeken Jan

Institution:

Ghent University

Research group / department:

WE05 / Center for Molecular Modeling

Title / position:

PhD student

email address:

jan.jaeken@ugent.be

Total computing time that is needed, in node days:

3106

Total disk storage that is applied for (in GiB):

1200 GiB SCRATCH, 100 GiB HOME

1. Title of the research project (with IWETO or FRIS link if available) within the framework of which computing time is applied for:

Mercury, the Earth, and exoplanets: the crystal structure and other properties of the inner core of terrestrial planets by Density Functional Theory and a genetic search algorithm

2. Describe your research project in short. Explicitly mention the scientific questions that you are planning to address and the overall scientific goals of the project. (max. 1 A4 in Arial 12):

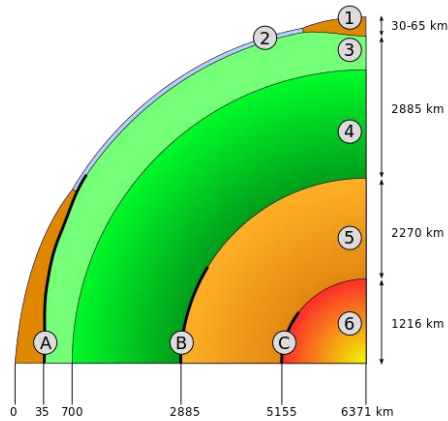


Fig. 1: Schematic view of the interior of Earth.

1. continental crust
2. oceanic crust
3. upper mantle
4. lower mantle
5. outer core
6. inner core

What we know of the inside of the Earth stems mostly from the study of seismic waves traveling through the planet with every earthquake. The specific velocities of these waves can tell us a great deal about the structure and composition of the layers deep within. The so-called inner core of our planet – a sphere with radius 1200 km -- consists mostly of iron, probably mixed with up to 10% Ni and minor fractions of other impurities. The crystal structure of this alloy is believed to be hexagonally close packed, probably with many defects. Key properties of this material when subject to the high pressure and high temperature of the inner core are not always accurately known. Indeed, these pressure and temperatures lie at the edge of what can be

recreated in a lab in order to measure these properties directly. This gets even worse when one wants to know the properties of the similarly built inner cores of Earth-like exoplanets (=planets in other solar systems), of which most of the presently discovered ones are heavier than the Earth. This leads to even larger pressures and higher temperatures in their inner cores.

Therefore, we take advantage of ab initio quantum simulations (in particular Density Functional Theory): the material is recreated in the computer, and its properties are determined by direct solution of the basic equations of quantum physics.

One important goal is to determine the elastic properties of defected Fe-Ni alloys as a function of pressure (extending beyond the pressure in the Earth's inner core). The full elasticity tensor of a material can be determined by quantum simulations, and we want to do that for pure Fe, pure Ni and a 50% Fe-Ni alloy. This allows to investigate the main trends over the Fe-Ni alloy series. For these three alloys, 6 typical crystal structures are considered: body centered cubic [bcc], face centered cubic [fcc], hexagonal close packed [hcp] and three stacking fault structures that are intermediate between fcc and hcp. The elasticity tensor is determined at 3 representative pressures. This gives eventually $3 \times 6 \times 3 = 54$ elasticity tensors, from which for

every material the resulting sound velocities and their anisotropies can be determined. This is crucial information for planetologists, who can use this information as input for full-planet models of the overall elastic behavior of the Earth and rocky exoplanets.

3. Provide an abstract (10 lines) for scientific communication on the website in layman's terms. See also item 13 of this application form.

What we know of the inside of the Earth stems mostly from the study of seismic waves traveling through the planet with every earthquake. The specific velocities of these waves can tell us a great deal of the structure and composition of the layers deep within. The inner core of our planet consists mostly of iron, though some uncertainties remain concerning the presence of impurities and the specific structure of the material at such pressures and temperatures. In this project, we use quantum simulations to determine sound velocities and their anisotropies for these Fe-based alloys under pressures that cannot be achieved in a lab. Planetologists can use this information for making better models of the elastic behaviour of the Earth and Earth-like exoplanets.

4. Financing institution or channel, financing the research project in full or in part (FWO, BOF, IWT, EU, ...): Please attach the confirmation letter as enclosure (see instructions in enclosure 4 "EasyChair proposals submission procedure").

FWO

5. Name and email address of the promoter(s) of the research project:

Prof. Dr. Stefaan Cottenier
Stefaan.Cottenier@UGent.be

Prof. Dr. Tim Van Hoolst (Royal Observatory Brussels)
Tim.VanHoolst@oma.be

6. Billing address to which the payment invoice will be sent to:

Jan Jaeken
Center for Molecular Modeling
T.a.v. Wim Dewitte
Technologiepark 903
9052 Zwijnaarde

7. Persons mandated by the Applicant to compute on the Tier1 within the framework of the present project: Please provide for every person:
 - name and first name
 - institution
 - research group / department
 - title / position

- experience of using HPC resources in the past (Tier0/Tier1/Tier2 infrastructure in Belgium and abroad)

M. Sc. Jan Jaeken (vsc40484)

Ghent University

Center for Molecular Modeling

PhD Fellow

Three years of experience with the VASP ab initio package on TIER2

Prof. Dr. Stefaan Cottenier (vsc40026)

Ghent University

Center for Molecular Modeling

Assistant Professor

Experience with a wide variety of DFT packages since the opening of the Ghent VSC on both TIER2 and TIER1.

8. Explain why this project needs to run on a Tier1 system, why the machine you have requested is suitable for the project and how the use of the system will enable the science proposed (max. ½ A4 in Arial 12).

The calculation of elastic parameters is done by studying several (up to 13) different deformations of the material, based on the symmetry of the crystal structure. For each deformation, 17 deformation steps are considered, each run as an independent calculation. This workflow benefits enormously from a highly parallel system.

Although some of the single calculations can be run on a TIER2 system, the enormous amount of jobs (nearly 10 000) combined with long wait times on smaller machines would make these calculations (especially the third stacking fault structure, see next paragraph) extremely cumbersome. Since the VASP k-point parallelization scheme scales very well in case of a modest (up to 10 nodes) multi-node approach, the TIER1 system is superbly suited for this task. It would allow to significantly push down computing time per job, while still running many jobs concurrently.

9. Justify the number of node days requested. This should include information such as: number and nature of computing tasks, software used, and the sequence in which they will be performed.
Indicate for each typical computing task the required resources:

- wall clock time (note that 3 days is the maximal wall clock time for any job; checkpointing should be used for longer run times)
- memory (maximum 64 GiB/node)
- number of nodes
- number of CPU cores
- disk space (estimated volume in GiB and the total number of files); make a clear distinction between usage of Tier2 DATA/HOME partitions and the Tier1 SCRATCH partition

- number of tasks, and an indication of how many such tasks would be submitted concurrently.

This information should take the form of a table (an example is provided as Table 2 in the appendix). Provide additional descriptions of the computing tasks and comments as needed. Resource estimates should be preferably based on the results of actual calculations on Tier1 (via, e.g., a Starting Grant) for system/problem sizes that are on par with those of the intended computing tasks (e.g., same mesh sizes, actual molecular system, ...). If not, provide the name, architecture, #cores, memory, etc. of the machine that was used to obtain these results and explain how you have calculated/rescaled the wall clock times, number of cores, etc.

(max. 1 A4 Arial 12).

For Fe, Ni and FeNi 6 different crystal structures are considered at 3 different pressures: Bcc, fcc, hcp and three close-packed stacking fault structures at 0, 50 and 345 GPa. The **memory** requirements of these calculations go up to **20 GiB/node** for the most demanding cases. Several test cases for Fe, Ni and FeNi have been considered on TIER2 to get an accurate estimate of the necessary computing time.

Computational task	Node day calculation			Storage volume est.	
	# of deformations x # of steps = # of tasks	# Tier1 node days per step	Total # node days	Perm volume (GiB)	Temp volume (GiB)
Fe stackfault 1	5 x 17 = 85	0.5	= 42.5	2	25
Fe stackfault 2	5 x 17 = 85	0.5	= 42.5	2	25
Fe stackfault 3	6 x 17 = 102	0.7	= 71.4	3	30
Ni stackfault 1	5 x 17 = 85	0.5	= 42.5	2	25
Ni stackfault 2	5 x 17 = 85	0.5	= 42.5	2	25
Ni stackfault 3	6 x 17 = 102	0.7	= 71.4	3	30
FeNi stackfault 1	5 x 17 = 85	1	= 85	2	25
FeNi stackfault 2	5 x 17 = 85	1	= 85	2	25
FeNi stackfault 3	13 x 17 = 221	2.5	= 552.5	6	65
Total			1053.3	24	275

Shown above are typical estimates for the resources needed to perform the calculations. The number of nodes per job varies due to symmetry considerations, yet the excellent scaling behavior of VASP ensures that only the total number of nodedays is relevant (see point 10). The highly symmetric crystal structures (bcc, fcc, hcp) are not included, as they only require around 10 nodedays in total. The stacking fault structures on the other hand, require significant more deformations and considerably more time per deformation step. Symmetry considerations will determine the optimal number of nodes per deformation, therefore only the total number of nodedays necessary per step are listed.

As each of these calculations will be run for three different pressures, the total computing time should be multiplied by three, giving a grand total of **1035.3 x 3 = 3106 nodedays**.

Per type of deformation for each stacking fault, it is best to have roughly 5 GiB of SCRATCH space available. The 3 low-symmetry crystal structures take up less than 1 GiB each. This totals to roughly 850 GiB. To prevent any storage issues, we suggest **1200 GiB SCRATCH storage**. For HOME storage, roughly 25 MB per step suffices, which totals to roughly 70 GiB. Therefore **100GiB of HOME storage** should be sufficient.

10. Describe the software required to perform the computing task(s). Please clearly provide the following per item in this regard:

- a reference to the software's web page
- the software license system (open source, GPL, etc.)
- if there is no free academic use of the software, state which license makes the installation and the use valid on the Tier1 by the Applicant (+ add a copy of the signed license)
- if need be, which license server will be used (name + IP address)
- whether the software is already available on the Tier1 (see <https://vscentrum.be/nl/Tier1-rekenen>) and, if this is not the case, compilation and installation instructions (possibly with reference to existing Tier2 installation)

Provide the results of scaling tests that were conducted with this software, preferably on Tier1 (using, e.g., a Starting Grant) for system/problem sizes that are on par with those of the intended computing tasks (e.g., same mesh sizes, actual molecular system, ...). If not, provide the name, architecture, #cores, memory, etc. of the machine that was used to obtain these results.

Provide both a table and scaling plot such as table 1 and plot 1 in the appendix (max. 2 A4 in Arial 12).

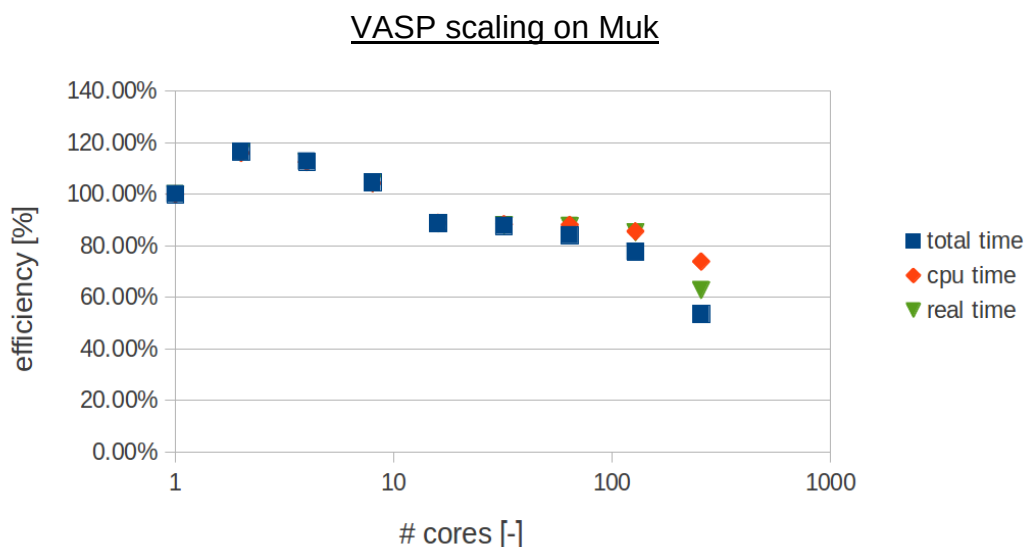
VASP

<http://www.vasp.at/>

non-exclusive academic licence (see attachment)
available on TIER1

Many scaling tests of the VASP software on Muk have been done in the past. For this project, k-point parallelization will ensure an efficient use of the computing facilities per job, while the ability to run many jobs concurrently will result in a timely completion of all necessary calculations.

The optimal number of nodes per job depends on the symmetry of the crystal, and the amount of symmetry breaking per deformation. These determine the number of irreducible k-points for the calculations, which are ideally distributed evenly across nodes, splitting the computational task in nearly serial parts. The jobs in this project would utilize up to 10 nodes (160 cores), ensuring an excellent scaling behavior, as shown below.



11. Describe how you will manage the resources requested in the period during which the task is to be performed. What usage pattern do you anticipate (similar usage on monthly basis, bursts, ...)?

The intention is to maintain a steady flow of jobs. Testing and preparation have been done, submission of jobs will commence as soon as the project is approved.

12. List the granted computing time allocations to the promoter(s) of this research project, on the Flemish Tier1 system, as well as other Tier1 and Tier0 systems. Also, describe the scientific output obtained within the framework of computing time that was granted during the past two years on the Flemish Tier1 or on other Tier1 or Tier0 supercomputers. DOI links are sufficient.

For this project, there have not been any calculations at the Tier1 level so far. However, the supervisor of the project and colleagues within the same group have considerable expertise in using VASP on the Flemish Tier1. Two examples:

Ab initio screening of suitable tungsten alloys as first wall material in nuclear fusion reactors (4000 node days)

Mechanical properties of lots of hypothetical binary and ternary tungsten-based alloys are calculated from first principles, in order to identify those alloys with the most suitable combination of properties to serve as a first wall component in future fusion reactors. Parts of this study have been published in the PhD thesis of Kurt Lejaeghere. New publications on a larger dataset are in preparation.

High-throughput determination of vacancy trapping enthalpies for the improvement of electronic device production (4420 node days)

Site selection and interaction with vacancies were calculated from first principles for 71 elements of the periodic table as impurity in the industrially important semiconductors Si and Ge. This leads to insight in the systematics of impurity-vacancy interaction, and complements the only partial experimental knowledge. Interpretation of this dataset allowed to single out a few impurity elements that can have a beneficial effect on lowering the vacancy concentration during germanium single crystal growth. A publication (first author Michael Sluydts) has been submitted.

13. Are the applicants of this application bound by a confidentiality agreement? If so, the title and the abstract of this application will not be published on the website of the Hercules Foundation / Flemish Supercomputer Center.

no

Should you have any questions or encounter any difficulties during the electronic submission of an Application, please contact by e-mail:
Associatie KU Leuven: hpcinfo@kuleuven.be
Associatie Universiteit Gent: hpc@ugent.be
Associatie Universiteit Hogescholen Antwerpen: hpc@uantwerpen.be
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SOFTWARE LICENSE AGREEMENT FOR THE USE OF VASP5.2 BY ACADEMIC INSTITUTIONS

The Universität Wien, Austria (UW in the following) and
Ghent University, Belgium (UG in the following) ¹
conclude the following agreement:

- (1) The UG acquires a non-exclusive academic license for the use of the software-package VASP (Vienna ab-initio simulationprogram) for ab-initio local-density-functional total-energy and molecular-dynamics calculations, **versions VASP5.2 and VASP4.6** by the research group Functional Nanomaterials (FUNNANO)². Under this licence the use of the software is restricted to a maximum of six researchers or students, all belonging to this research group and to the same organisational unit and working at the same location. The licence does not cover the use of VASP by external collaborators working at other institutions.
- (2) The license covers access to the source-code, the program documentation and to the data-base for ultrasoft pseudopotentials and PAW-potentials. UW reserves the exclusive property of the software. It declines any liability for the software and any responsibility for the results of calculations produced with the program. The license does not cover any maintenance service for the software or support for its implementation.
- (3) The license is not transferable to another research group of UG without the written agreement of UW. UW reserves the right to refuse authorization of such a transfer. A transfer to a research group not belonging to UG is excluded.
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¹Please insert here the name of the institution concluding this agreement with UW. This institution must be a legal person and the agreement must be signed by an authorized representative of this institution. Define the acronym (replacing) under which this institution is referred to in the text of the agreement.

²Please insert here the name and affiliation research group for which the license is acquired

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(5) If VASP is used as the basis of further methodological or software-development, UG agrees to make these additions available to UW. UW will also be entitled to include these additions in further releases of VASP.

(6) In future publications of work performed using VASP, the use of the software shall be properly acknowledged, e.g. in the form

”The calculations have been performed using the ab-initio total-energy and molecular-dynamics program VASP (Vienna ab-initio simulation program) developed at the Institut für Materialphysik of the Universität Wien [1-3].”

[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11 169 (1996).

If the PAW-version is used, reference will be made to

[2] G. Kresse and D. Joubert, Phys. Rev. **59**, 1758 (1999).

If special features implemented in VASP will have been used, reference should be made to the relevant publications as listed on the VASP home-page.

(7) The UG accepts to pay to UW a licence fee Euro 4.000,- (fourthousand Euro). The licence fee is strongly discounted and applies only to academic institutions with undergraduate teaching.

(8) The licensee will use VASP exclusively for non-profit research. If VASP is used in contractual research in cooperation with or for industry or for military institutions, the financial conditions will have to be re-negotiated.

(9) UW declares that it has the full power and authority to grant the rights granted in this agreement without the consent of any other person, and that the license and use of the software by the licensee will not in any way constitute an infringement or other violation of any copyright, proprietary right or any other rights of any third party.

(10) Any disputes arising from the license agreement are subject to the laws of the Republic of Austria.

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For the Universität Wien:

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Date

For the UG

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Address: Technologiepark 903, BE-9052 Zwijnaarde, Belgium

Date: 26 January 2010

For the research group entitled to use VASP5.2:

Name (in print): Veronique Van Speybroeck (FUNNANO)