



IAEA

International Atomic Energy Agency

Atoms for Peace and Development

INVITATION TO AN IAEA CHALLENGE

MODELLING DAMAGE IN A FUSION REACTOR

REF.: 120285-SA

NEW CLOSING DATE AND TIME:

14 JULY 2018

17:00 HOURS CET (VIENNA, AUSTRIA, LOCAL TIME)

1. BACKGROUND

The International Atomic Energy Agency (IAEA) is the world's central intergovernmental forum for scientific and technical co-operation in the nuclear field. It works for the safe, secure and peaceful uses of nuclear science and technology, contributing to international peace and security and the United Nations' Sustainable Development Goals. More detailed information about the IAEA can be found at <https://www.iaea.org/>.

2. THE CHALLENGE: MODELLING DAMAGE IN A FUSION REACTOR

Nuclear fusion is the process by which the nuclei of two light atoms combine to produce a single nucleus whilst releasing a large amount of energy. A star like our own Sun shines because of energy released from a set of fusion reactions which convert hydrogen to helium.

A nuclear fusion power station would have many advantages over the nuclear *fission* reactors currently in use across the world (nuclear fission is the process of splitting heavy atoms of uranium or plutonium to release energy). A fusion reactor has the potential to produce cheap, clean energy without the dangers of long-lived radioactive waste or weaponisation.

In order to get two nuclei to fuse, they have to hit each other at immense speed (since both are positively-charged, there is a strong electrostatic repulsive force between them). In most designs of experimental reactor, the nuclei involved are two isotopes of hydrogen, deuterium (^2D) and tritium (^3T) which combine at a temperature of 100 million $^{\circ}\text{C}$ to form a helium nucleus (^4He) and release an energetic neutron (^1_0n):



At such high temperatures, matter exists as a *plasma* of positively- charged nuclei and negatively-charged electrons. This plasma must be confined by a magnetic field to keep it from damaging the reactor walls and the details of maintaining a stable plasma confinement are the subject of ongoing research.

A further obstacle to a practical fusion reactor design concerns the neutrons which carry most of the energy which will ultimately drive turbines to produce electricity. Being uncharged, they are not confined by the magnetic field but pass through the reactor “first wall” to deposit their energy in a specially-designed “blanket” which efficiently slows them, releasing their kinetic energy

This challenge is concerned with the material that might make an effective first wall: in the extreme environment near to the fusion plasma, such a material is exposed to high temperatures and bombardment by the highly-energetic neutrons and other particles. Candidate materials include tungsten, steel and beryllium. Since experiments on physical samples are difficult and expensive to carry out, scientists have turned to computational models to simulate the behaviour of a material.

Molecular Dynamics is the method used to simulate the physical movement of the atoms in a solid material after the disruptive impact of a high-energy particle such as the neutron resulting from a fusion reaction. This impact can be profound for a local region of the material, creating a *cascade* of displaced atoms and creating voids, defects and dislocations in its structure. By following the movement of the atoms in the material, the damage created can be simulated and analysed. Different metals or compositions, impact energies and temperatures can be explored in this way and can help with the search for an effective first wall material.

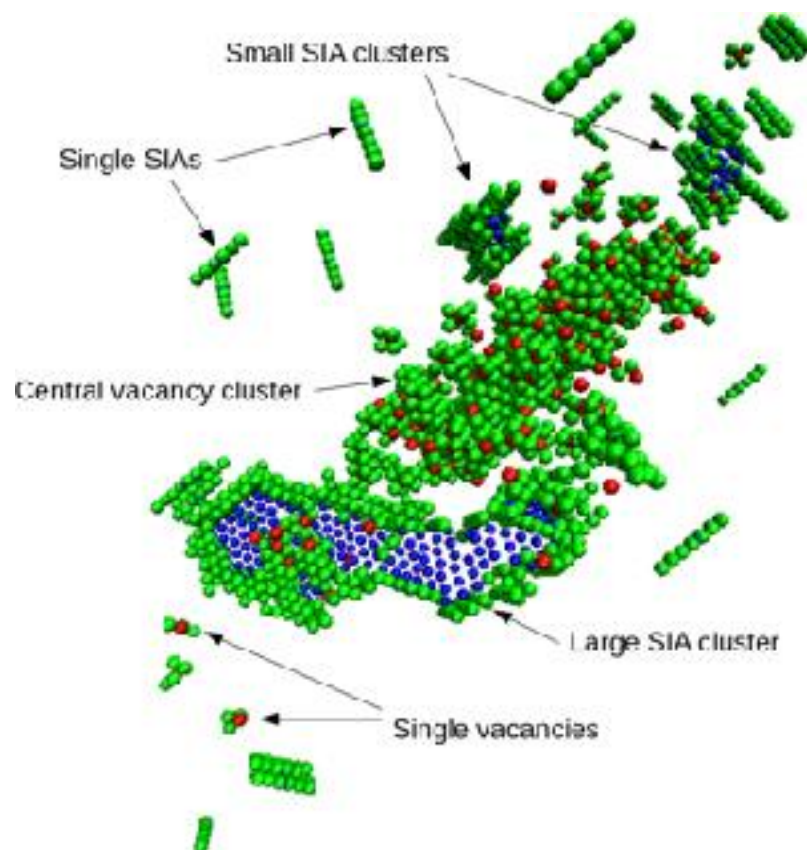


Image: The final damage configuration from an impact event, visualised using conventional methods. A. E. Sand *et al.*, *J. Nucl. Mater.* **455** (2014) 207–211.

3. THE CHALLENGE

The IAEA invites interested parties to participate in the challenge for “Modelling damage in a Fusion Reactor” (the “Challenge”).

Participants are invited to come up with novel ways to visualise, analyse and explore the provided data. The precise nature of the software solution to the challenge is deliberately left open to invite as many novel approaches as possible, but may involve one or more of the following:

- Novel software for visualizing the material damage represented by the data files in a way that aids its qualitative and quantitative assessment.
- New software tools to rapidly and reliably identify, classify and quantify new patterns and structures of particular kinds in the data sets.
- Efficient algorithms to depict and summarise the statistical distribution of atom displacements and to analyse the effect of impact energy on this distribution.

It is envisaged that analysis techniques applied in the domains of tomography, medical imaging, protein crystallography, computer vision may be applied in a modified form to address the proposed Challenge.

4. THE IAEA DATA DESCRIPTION

The data files for this Challenge may be obtained from <https://int-amdis.iaea.org/CDB/challenge/>.

The metadata associated with each file is accessible in the same location in XML format. An XML Schema document against which the metadata files may be validated is also available there, along with human-readable versions (in text and HTML).

The data provided are the positions of the atoms of either tungsten, W, or iron, Fe, after a collisional cascade molecular dynamics simulation run for 40 picoseconds. The initial state of the material is taken to be a perfect crystal, and the final state is provided as the (x, y, z) locations of the atoms after the energy of the impacting neutron has been absorbed. Four different impact energies are considered for each material and at least seven different simulations are run (for different impact directions) for each energy.

5. DELIVERABLES

Participants shall provide the following deliverables by the challenge end date:

- A completed solution description form (obtainable through the challenge website, <https://challenge.iaea.org/>) outlining their analysis of the data and explaining the technical, mathematical or algorithmic approach to their solution.
- The means to obtain a working executable version of the software developed, with full instructions for its compilation (if appropriate), installation and deployment.

Submissions utilising open source technologies are particularly encouraged.

- A well-described test suite of example input files to the submitted software application and their expected outputs.

6. PRIZE

The participant (be it an individual a team or legal entity) with the best submission, as judged by the advisory panel, will be awarded €5,000 and invited to the IAEA Headquarters in Vienna, Austria to present their solution.

7. GENERAL REQUIREMENTS FOR THE CHALLENGE SUBMISSION

- a) The Challenge is open to individuals, teams, companies, non-commercial organizations and other organisations in any Member State of the IAEA.
- b) The Challenge submission shall be in English.
- c) Illustrative materials including videos, charts, diagrams, figures and other illustrations accompanying the submitted software are to be subject to the Creative Commons BY-SA (Attribution and share-alike) License allowing royalty-free reuse.
- d) Each Challenge submission is to be uploaded as a single zip or tar archive to a URL advised on submission of a completed form at the challenge website. tar archives may be compressed with gzip or bzip2.
- e) Submissions must contain a completed solution description form (obtainable through the challenge website) outlining their analysis of the data and explaining the technical, mathematical or algorithmic approach to their solution.
- f) The software for solving the Challenge should be operable under one or both of the Microsoft Windows or Linux operating systems. Full and clear instructions for its deployment and testing must be provided. The submission of code released under an open-source software licence is particularly encouraged.
- g) A well-described test suite of example input files to the software application and their expected outputs should be provided with the submission.
- h) The language of the Challenge is English. Where translations into other languages are provided they are for guidance only and the English description, regulations and procedures are to be considered normative and shall therefore prevail. Requests for clarification or further information concerning the Challenge must also be submitted in the English language.

8. TIMETABLE, EVALUATION AND JUDGING

- **26 April 2018** **Challenge opens**

Participants register at <https://challenge.iaea.org/>, indicating their intent to participate in the challenge and providing their contact details. Registered participants will have access to a page providing additional relevant details and instructions. This page also provides the participants the possibility to send clarification questions; the IAEA will answer these and regularly update a FAQ list until the close date and time of the challenge to ensure that all participants have the same information.

- **14 July 2018** **Challenge closes**

Participants shall provide the deliverables described above in a suitable form by this date.

- **July – August 2018** **Evaluation and Judging**

Submissions will be evaluated and, where appropriate, compared by the advisory panel. Code provided may be executed on further data sets of simulated material damage. The following criteria will apply:

- i. Scientific correctness, as benchmarked against existing software tools;
- ii. Visual impact in the depiction of important features in the data;
- iii. The innovative, efficient and effective application of algorithmic analysis techniques to the data;
- iv. Conciseness, ease of deployment and use.

- **15 August 2018** **Winner announced**

The winning party will be contacted, and an announcement made online and through the IAEA's public communication channels. The winner will be invited to IAEA Headquarters in Vienna to present their solution.

9. GENERAL REQUIREMENTS

- a) The IAEA reserves the right to request any additional information or documentation and to verify the information provided in the Challenge submission.
- b) All Challenge participants shall adhere to the highest ethical standards.
- c) This Challenge is not a solicitation and does not entail any commitment on the part of the IAEA, as such, this Challenge announcement does not commit the IAEA to finalize this process. Any Challenge submission will be regarded as a submission and not as an acceptance by the participant of any kind of offer from the IAEA.
- d) Any and all costs and expenses incurred in relation to, or ensuing from, the Challenge submission will exclusively be borne by the participants. The Challenge submission

will not be subject to claims for financial compensation of any kind whatsoever regardless of the outcome.

- e) The IAEA reserves the right to reject any or all the Challenge submissions without incurring any obligation to inform the affected parties of that decision or the grounds thereof and/or change or cancel this process at any time.
- f) Information relating to the examination, clarification, and evaluation of the Challenge submissions shall not be disclosed.