Institution: Queen Mary University of London		
Unit of Assessment: 9		
Title of case study: State-of-the-art algorithms for modelling radiation damage change international policy on managing nuclear safety		
Period when the underpinning research was undertaken: 2010–present		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Prof. Kostya Trachenko	Professor of Physics	Jan 2010–present
Period when the claimed impact occurred: 2013–present		
Is this case study continued from a case study submitted in 2014? N		

1. Summary of the impact (indicative maximum 100 words)

Queen Mary's Prof. Trachenko has developed innovative radiation modelling algorithms and implemented them in the leading software framework DL_POLY. Trachenko's molecular dynamics code is the first in the world to provide on-the-fly modelling of the damage that radiation imparts to a given material. By eliminating computational bottlenecks including large file sizes, Trachenko's high-performance algorithms are able to model very large systems and high-energy collisions, creating for the first time realistic models of real-world nuclear encapsulation materials. This innovation is of significant global importance given the damaging consequences of radioactive waste and unstable reactor cores. The code has informed international policy on nuclear materials and waste storage at the US Oak Ridge National Laboratory, the UK National Nuclear Laboratory and the UK Nuclear Decommissioning Authority. The United Nations has used Trachenko's algorithms to define best practice for the safe disposal of nuclear waste for its 193 Member States, while the UK Atomic Weapons Establishment has used them to improve its storage of nuclear materials, and to streamline working processes.

2. Underpinning research (indicative maximum 500 words)

Despite its potential value as a reliable source of low-carbon energy, the safe and effective implementation of nuclear power presents major challenges. Spent fuel from fission reactors remains highly radioactive for hundreds of thousands of years, and therefore requires suitable containers in which to bury this potentially damaging waste, while the metals required for fusion reactor cores must be structurally stable enough to withstand extreme conditions.

Research by Queen Mary's Prof. Trachenko has made crucial contributions to resolving these issues by enabling relevant materials and scenarios to be realistically modelled for the first time [3.1–3.4]. By moving from "post mortem" analysis to an on-the-fly approach to modelling, Trachenko's work has overcome two computational bottlenecks in the classical molecular dynamics simulation software DL_POLY, originally developed at Daresbury Laboratory by I.T. Todorov and W. Smith, and currently maintained by the UK Science and Technology Facilities Council (STFC). Previously, DL_POLY was unable to efficiently simulate or analyse very large systems and lacked the necessary algorithms for dedicated radiation modelling.

Trachenko designed algorithms to handle large systems on the fly using a 'variable timestep' method. Timesteps are the incremental intervals over which the equations governing a system are solved for a scenario in which parameters change unevenly with time, such as radiation modelling. At each simulation step of a system, the maximum distance travelled by a particle is used to define and reset the timestep, allowing the simulation to slow down enough to accurately model the dynamics at the most violent stages of a nuclear collision, and then speed up again to utilise CPU time most effectively when the system cools. The simulations also provide more effective energy dissipation and faster temperature relaxation, via a 'thermostat bath', which in turn accelerates modelling and allows the simulation of higher-energy impacts. Furthermore, Trachenko designed an efficient defect detection tool that compares the data in a given simulation to reference data for the same material in its undamaged state in order to efficiently ascertain the number of defects and, hence, the amount of radiation damage that a material has suffered (Fig. 1). Trachenko has also adapted numerous other recent pioneering radiation modelling ideas, such as Duffy and Rutherford's electronic energy loss algorithms, and incorporated them into his on-the-fly approach to simulation.

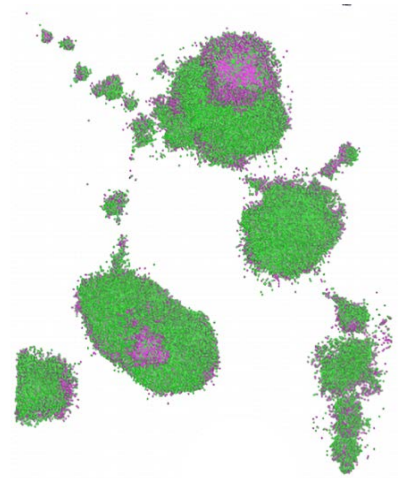

Figure 1: Radiation damage in iron from a parallel DL_POLY simulation using 500 million atoms. Different types of defect are shown in green and purple; undisturbed atoms are not shown. Figure reproduced from [3.1]. Copyright [2013].

More recently, Trachenko has focused on implementing these algorithms in collaboration with the developers of DL_POLY [EQR. 1]. The completion of this grant provides a proof of principle that on-the-fly algorithms not only work, but can also successfully replace post-mortem analysis, saving valuable expert time in interpreting simulation results.

3. References to the research (indicative maximum of six references)

[3.1] E. Zarkadoula, S. L. Daraszewicz, D. M. Duffy et. al. The nature of high-energy radiation damage in iron (2013). *Journal of Physics: Condensed Matter*, *25* (12). http://dx.doi.org/10.1088/0953-8984/25/12/125402.

[3.2] E. Zarkadoula, S. L. Daraszewicz, D. M. Duffy et. al. Electronic effects in high-energy radiation damage in iron (2014). *Journal of Physics: Condensed Matter*, *26* (8). http://dx.doi.org/10.1088/0953-8984/26/8/085401.

[3.3] E. Zarkadoula, D. M. Duffy, K. Nordlund et. al. Electronic effects in high-energy radiation damage in tungsten (2015). *Journal of Physics: Condensed Matter*, *27* (13). http://dx.doi.org/10.1088/0953-8984/27/13/135401.

[3.4] E. Zarkadoula, R. Devanathan, W. J. Weber et. al. High-energy radiation damage in zirconia: Modeling results (2014). *Journal of Applied Physics, 115* (083507). https://doi.org/10.1063/1.4866989.

Evidence of the quality of the research:
[EQR. 1] PI, K Trachenko (Oct 2011–Sept 2013). Developing DL_POLY Molecular Dynamics Simulation code to tackle challenging problems in science and technology [EP/I029311/1]. *EPSRC*. Research Grant. GBP35,000.

[EQR. 2] PI, K Trachenko. (Dec 2017–Dec 2020). Modelling of glasses as nuclear waste forms [EP/R004870/1]. *EPSRC*. Research Grant. GBP367,991.

4. Details of the impact (indicative maximum 750 words)
The state-of-the-art algorithms developed by Queen Mary's Prof. Trachenko, incorporated into the leading software DL_POLY, have been used

- to inform policy and choice of materials for radioactive waste storage by leading international organisations
- to assess and safeguard the UK's nuclear deterrent through adoption by the UK government
- to significantly enhance the international reputation and competitiveness of Daresbury Laboratory and the UK STFC as the UK hub for computational science and engineering

For his work on DL_POLY, Trachenko was awarded the 2020 EPSRC-funded Collaborative Computational Project (CCP5) Prize and Lecture, given biennially to an outstanding UK or overseas scientist in the field of classical molecular simulation [5.1].

Informed vital national and international policy on radioactive waste storage
Trachenko's code enables researchers to efficiently determine the defects in a material and model the radiation damage which that material can handle before becoming unstable. This is essential for identifying materials that are suitable and able to safely encapsulate radioactive nuclear waste. The algorithms have been used by numerous leading organisations in the UK, US and internationally.

US Oak Ridge National Laboratory
The US Oak Ridge National Laboratory (ORNL, the largest of the US Department of Energy's science and energy laboratories) used Trachenko's algorithms to run detailed radiation damage simulations. According to William Weber, Governor's Chair Professor, University of Tennessee Knoxville, the ORNL has used DL_POLY "to run detailed radiation damage simulations, with a view to finding new suitable materials for radioactive waste storage and radiation tolerant high-entropy alloys for nuclear fission and fusion energy systems" [5.2]. Professor Weber affirms that the radiation damage modelling features implemented in DL_POLY as a direct result of Trachenko's contributions "are unique to the package and include the ability to model high-energy collisions, accurately detect defects and model large numbers of atoms in a way that would simply not be possible using other available software or earlier versions of DL_POLY" [5.2]. DL_POLY is now the laboratory's "preferred software for modelling complex ceramic materials" with "the implementation of the two-temperature model approach in DL_POLY being far superior to that in previously used software." Much of what the laboratory has accomplished would not be possible without the use of DL_POLY [5.2].

UK National Nuclear Laboratory
The UK National Nuclear Laboratory (NNL), which advises the Nuclear Decommissioning Authority (NDA), have a particular interest in the use of ceramics as casing materials for radioactive waste and have joint-funded PhD studentships using DL_POLY to explore how the decay of encased radioactive material, for example plutonium, damages ceramics. This is "very relevant to the UK's large plutonium stockpile at Sellafield, Cumbria" [5.3].

United Nations International Atomic Energy Agency
The United Nations International Atomic Energy Agency (IAEA) has been significantly influenced by Trachenko's results. In 2016, the IAEA organised a joint workshop with the International Centre for Theoretical Physics (ICTP) in Trieste, Italy, on *Radiation Effects in Nuclear Waste Forms and their Consequences for Storage and Disposal.* As Mr Danas Ridikas, Section Head, Physics Section, Department of Nuclear Sciences and Applications at the IAEA says, this workshop was aimed at "bringing the state-of-the-art" to scientists "particularly from developing countries." The IAEA contacted Trachenko as he is "an internationally recognised expert in developing and applying the molecular dynamics code DL_POLY to such problems" [5.4]. The IAEA also appreciated the freely available nature of his software as this ensures results "can be be easily shared with many other groups around the world." Following the meeting, the IAEA created a new *Coordinated Research Project (CRP)* designed to "address themes of current interest in radiation and nuclear sciences" and to "bring together experts from around the world, both from developed and developing countries." Prof. Trachenko was brought in as a Chief Scientific Advisor due to his "expertise as the key developer of the radiation modelling aspects and approaches" and to his "long-lasting experience in usage of … state-of-the-art software." In a "largely experimental CRP, Prof. Trachenko and his group ... became indispensible contributors providing the simulation work" [5.4]. The IAEA will publish the results of this collaboration in a Technical Document (TECDOC), "available at no cost to all IAEA Member States with the aim to document and disseminate the state-of-the-art in these technical areas." [5.4].

Safeguarded the UK's nuclear deterrent via critical assessment of warhead safety
The UK Government's Atomic Weapons Establishment (AWE) is "responsible for manufacturing, maintaining and developing warheads for the UK's nuclear deterrent" [5.5]. The new radiation modelling features in DL_POLY are "invaluable to the AWE, which carries out a range of experimental and theoretical research into the ageing of radioactive materials such as metals and oxides." Prof. Mark Storr of AWE comments that "Understanding the ageing process is vital to designing the optimum storage conditions and environment [for radioactive materials]. This is where the DL_POLY software plays a key role." Furthermore, use of DL_POLY "reduces the number of experiments needed, thereby cutting costs and speeding-up research" [5.5].

Enhanced the expertise and competitiveness of the STFC and Daresbury Laboratory
The DL_POLY software package, a "UK flagship project" owned by the STFC and distributed solely by the Daresbury Laboratory since 1993, has been significantly improved and extended by Trachenko's algorithms, according to Head of Computational Science and Engineering at STFC, Dr. Barbara Montanari [5.6]. She says, "Prof. Trachenko's methods have allowed DL_POLY both to simulate very large systems for the first time, and to efficiently include the effects of very high energy collisions. Not only does this allow for the modelling of radiation damage in materials, but this was also the first molecular dynamics code available in the world that could do so". As a result, "both Daresbury Laboratory and the UK STFC significantly enhanced their international reputation and competitiveness as the UK hub for computational science and engineering" [5.6]. The new features have been distributed to 3,000 global users, including 500 in the UK.

5. Sources to corroborate the impact (indicative maximum of 10 references)

[5.1] K Trachenko (2020). Collaborative Computational Project (CCP5) Prize and Lecture. *EPSRC*. The award is given biennially to an outstanding UK or overseas scientist in the field of classical molecular simulation. https://www.ccp5.ac.uk/prizes.

[5.2] W. J Weber. Governor's Chair Professor. *University of Tennessee Knoxville* (testimonial letter, 27 May, 2020). [Corroborator 1]

[5.3] Palmer, N. A., Read, M. S. D., & Elena, A. M. (2018, January 17). *Computational modelling of PuO2 ageing and fuel residues*. Nuclear Decommissioning Authority PhD Research Seminar for NDA-Sponsored PhD Projects. Manchester Conference Centre.

[5.4] D Ridikas. Physics Section Head. *IAEA* (testimonial letter, 21 May, 2020). [Corroborator 2]

[5.5] O'Sullivan, M. & Geatches, D. (2020, July 27). *Simulation software fuels workflow efficiency in the nuclear industry* [STFC Case Study]. Ministry of Defence © British Crown Copyright 2020/AWE. https://www.scd.stfc.ac.uk/Pages/Simulation-software-fuels-workflow-efficiency-in-the-nuclear-industry.aspx

[5.6] B Montanari. Head of Computational Science and Engineering. *STFC* (testimonial letter, 28 May 2020). [Corroborator 3]