

eIUS Use Cases

In these examples, underlined elements are based either on the original interview data or on feedback sent by the informants in response to draft versions of the use cases. Key activity types are highlighted in italics and relevant ICTs in bold.

Use Case 15 – Microelectronics

Narrative

1. Robert is a researcher at a leading electronics department at a UK University. In a project including a number of partners from other national universities and the semiconductor industry he is working on large-scale simulations of transistors to improve the design of future microchips.
2. Bill is working for a semiconductor company which is a collaborator in the project. As transistors get smaller and smaller their characteristics are affected by the positioning of individual atoms. Bill hopes that Robert's high performance computing simulations at the quantum level will help to *predict the performance of transistors on a chip* (there may be up to several billion transistors on one microchip), e.g. to simulate their reliability or power efficiency.
3. To test one of their latest microchips on its power efficiency Bill sends Robert data on the transistor architecture and a file with its physical specifications (**spec file**). Robert as usual starts his day in the office by going through his email and saves the files from Bill's message on his computer. He looks at architecture and specifications of the transistor and starts preparing the simulation with the aim of generating characteristics to measure power efficiency.
4. Before running the simulation Robert *checks on the relevant latest literature, something he does regularly as the field moves very quickly.* He starts his browser and logs in the **Xplore portal** to skim through the articles of the most prominent **IEEE journal** in the field, '**Transactions on Electron Devices**'. He then downloads two papers and has a closer look at them, collating some information which is relevant to the simulation.
5. Later that day Robert *configures the parameters of the simulation software* and feeds in the transistor **spec file** Bill sent him to *create his simulation model.* The **simulation software suite** he uses has been developed during the project and enables the *use of high performance computing over the Grid.* Robert *opens the job submission tool **Ganga** to start his simulations on the **ScotGrid**,* as he needs all the resources he can get to *run a few thousand simulations to generate collections of current-voltage characteristics, a basic parameter to find circuits which are low in power consumption.*

6. During the course of the simulations Robert *uses Ganga* to occasionally check on his running processes on the **ScotGrid**. Eventually all simulation runs are completed and the collected data – a couple of thousand result files, at least one for each transistor and simulation – is stored in a database on a secure server.
7. Robert *accesses the data* and begins to *analyse* it on a set of parameters which might influence power efficiency. To this end he writes his own code using the **R** and **Python** programming environments on his desktop computer. He then runs data mining and statistical operations on the data to extract the characteristics he is looking for and subsequently collates his findings. After looking at the findings Robert is unsure about the relevance of one specific parameter in the simulation model. To get a second opinion he zips and emails a small subset of the data to his colleague Sonya who is an expert in current-voltage characteristics and works in the project in a research group at another UK University.
8. Having received the **zip-file** via **email** in her office Sonya checks the data and comes to the same conclusions as Robert. With **Skype** already running on her computer she sees Robert is online and calls to reassure him. During the call both also agree on submitting an article on the topic in the **IEEE journal** on ‘**Electron Device Letters**’.
9. After having fully completed his analysis, identifying the relevant characteristics for achieving power efficiency Robert goes over to visualise the data which is of interest for the chip manufacturer. Using the tools **Grace** for **2D plotting** and **OpenDX** for **3D visualisation** Robert creates a report depicting his findings, especially pointing out how the actual physical properties of the transistors in the simulations result in low power consumption.
10. Robert emails the report to Bill, who is very pleased to find useful results for his company’s next evolution of microchips.
11. Robert and Sonya continue *collaborating* on their journal article via **email**, **Skype** and telephone calls until they submit their final version. A few months later they have their article accepted for the next issue of ‘**Electron Device Letters**’.

Relevant ICTs

ICT	Comments
Spec file	The spec file is a plain text file containing the specification of a transistor. It is required by the simulation software which needs parameters of the transistor's actual physical construction for a proper simulation.
IEEE Journals available on the IEEE Xplore online portal ¹	The IEEE Transactions on Electron Devices ² journal is the most important in the domain, followed by the IEEE Electron Device Letters ³ . Both are available online through the IEEE Xplore portal via subscription.
Simulation software and Grid-enabled infrastructure	The project developed a grid-enabled atomistic device simulation service (integrating diverse simulation tools developed for different tasks) within a grid-enabled simulation framework. Currently computer cluster at the university's electronics department or for larger simulations the ScotGrid ⁴ including the job submission and management tool Ganga ⁵ are used. A secure webpage and encrypted file system are used for direct input into the simulation software.
R ⁶ and Python ⁷ used for data analysis	R is an open programming language and powerful statistical package. Python is an open source programming language applicable for various software development purposes which supports interoperability with other tools and languages. Using these software packages also means that a lot of code has to be written by the researchers for every new simulation and analysis model.
Grace ⁸ and OpenDX ⁹ visualisation software	Grace is an open visualisation tool used for 2D plotting while OpenDX can be freely used to visualise data in 3D.

1 <http://ieeexplore.ieee.org/Xplore/dynhome.jsp>

2 <http://www.ieee.org/ted/>

3 <http://www.ieee.org/edl/>

4 <http://www.scotgrid.ac.uk/>

5 http://www.scotgrid.ac.uk/wiki/index.php/Ganga_Quickstart_Guide

6 <http://www.r-project.org/>

7 <http://www.python.org/>

8 <http://plasma-gate.weizmann.ac.il/Grace/>

9 <http://www.opendx.org/>

Commentary

Protagonists: This case study narrative is based on interviews with two researchers from the project. **Security, IPR and Grid:** IPR issues (sensitive data) sometimes make it difficult to run jobs/simulations on the NGS or ScotGrid as the security/ authentication framework is under development as one of the project's main goals (standards like the Kerberos protocol, Andrew File System (AFS) and Shibboleth is/will be used). In such cases the computer closed cluster in electronics (University Institute) is used. In this context a production level service for job submission is under development as well.

Data: Ways of proper data management have become essential due to the rising number of data files coming out of the simulations. Currently there are no common standards for metadata used in the field, besides for some basic metadata (which simulation, run by whom, when, where) – this might not change, as the more complex metadata varies and is different for every simulation and transistor.

Collaboration: There are different groups in the project with different expertises which makes knowledge transfer within the project important. Weekly meetings in at one institution are followed by weekly management telephone conferences with the project partners and also sometimes bilateral meetings. Occasionally AG, f2f meetings and Skype is used as well.

Dissemination: More and more publications in the field also publish parts of the results along with the paper – not necessarily raw data, but e.g. summary tables with important detail information.

Other Editorial Considerations

Element	Usage
Links to direct quotes?	No
Year?	No
Month?	No
Time of day?	No
Location given?	No
Real institutions named?	No
Real journals named?	Yes
Real conferences named?	No