MDENet | The home of model-driven engineering

MDENet thematic workshop on Research Software

MDENet, the expert network for model-driven engineering, are pleased to invite expressions of interest to attend the fourth thematic workshop, addressing the intersection of model-driven engineering (MDE) and research software.

MDENet thematic workshops aim to improve mutual understanding of research challenges and opportunities for MDE to help address problems in a particular thematic area or for insights and expertise from a thematic area to contribute to the development of MDE. Our goal is that the workshop can spark collaborations between people in different areas. MDENet offers a range of funding opportunities to support the further development of such collaborations.

Many areas of research involve developing complex bespoke software – ranging from simulations, HPC calculations and analysis, to device control software etc. The need to deliver scientific outcomes creates pressure to "just build" and sound software engineering principles can be more challenging to adhere to. This is exacerbated where software is developed by experts in the sciences who may not necessarily have a software-engineering education. This can lead to challenges in maintainability, reproducibility, robustness, and reliability of the software developed and scientific results that depend on it. Over recent years, there has been a growing interest in developing a community of research software engineers to address these challenges. Research software engineers (RSEs) bring software-engineering expertise to the development of complex research software.

Model-driven engineering (MDE) is a subfield of software engineering providing techniques and methodologies for addressing complexity and scale in software development and enabling stakeholders with different expertise and background to collaborate fully in the development of software. It does this by developing software from high-level models expressed in domain-specific modelling languages (DSMLs) and translated automatically into executable code. DSMLs are formal languages based on concepts of the problem domain, enabling direct expression of a stakeholder's problems into software. Automated translation of models written in a DSML means that the translation programs become explicit artefacts themselves that can be inspected, tested, improved and extended over time. DSMLs thus can help manage the complexity of a domain while automated translations can contribute to reproducibility, robustness, and can enable research software to be validated more directly from a problem-domain perspective (cf also https://ieeexplore.ieee.org/document/9622288 for an exploration of the V&V challenges in the development of scientific software).

Examples of where MDE approaches have been successfully applied to scientific software include:

1. Citizen Science: In an ongoing MDENet seedcorn fund project, researchers from Aston University and the University of York have worked with Earthwatch Europe to define a DSML for describing the data management practices of citizen science projects. They have implemented a DSML following the ISO 19115-3 data lineage concepts, with automated generation of HTML reports. Writing in the DSML looks like filling in a document-based form, while more rigorously enforcing the ISO 19115 standard and providing automated live validation.

   In the future, this DSML could also automatically produce machine-readable versions to allow for interoperability with citizen science data repositories, e.g. ISO 19115's XML Schema-based format. The research team is currently conducting a user study with citizen science project coordinators to evaluate the usability of the DSML and prioritise further work.

2. Multi-physics simulations. Researchers and engineers can create very complex multi-physics simulations via model-based software. Popular software examples are Comsol Multiphysics

and Lumerical. For instance, Comsol offers a model editor that allows combining CAD-based geometry modelling, physics-based modelling, and/or equation-based modelling to simulate and analyse complex systems or materials, such as optical constants or thermal properties. This software also helps with model validation, with the process of persisting and versioning models, and with the deployment of applications based on the defined models.

3. Simulator development in computational biology. Computational biology develops simulators to study hypothesised mechanisms. These are typically developed in general purpose programming languages, creating challenges for validation, reuse, and maintenance. Using DSMLs, it is possible to develop simulations more closely linked to the scientific understanding, helping to alleviate these concerns.

4. Managing HPC pipelines. HPC pipelines and scientific computations are complex systems and require careful management. MDE and DSMLs can help manage this complexity, identify errors, and support corrective action.

MDENet thematic workshops are aimed at both an academic (MDE experts and research software experts) and an industrial audience (research software experts at management, research and development level). Participants are invited to bring to the workshop problems in research-software development as well as MDE research challenges, but initial ideas for potential solutions are also welcome.

During the day, we will begin with a brief round of introductions and then, after a keynote talk, we will then identify themes and sub-groups. This will help us identify specific themes of interest to be further refined and discussed in more depth in various smaller-group discussions.

A key goal of MDENet thematic workshops is to support the seeding of new collaborations. Therefore, a substantial amount of time will be spent on discussions between participants following the initial presentations, as well as in breakout groups.

The expected outcomes to be yielded from our thematic workshops range from seedcorn proposals (two submitted from previous MDENet thematic workshops) – that arise from the discussions on working groups, bridging some areas and coming up with new collaborations – a short report summarising the discussions had throughout the event (previous reports can be found here) and, informally, the links that people have made, getting to know other attendees and talking amongst them.

Participants will be able to apply to our Seedcorn Fund, to provide support for developing initial ideas from the workshop into new collaborations and research projects.

The thematic workshop will take place on October 31st and will be an in person event at King's College London.

Expressions of Interest

At this point, we are inviting short expressions of interest to ensure a diverse group of participants that will be able to effectively collaborate as part of the workshop. To submit an expression of interest, fill out this form.

Expressions of Interest will be reviewed by a participant selection panel to ensure a diverse and broad group of participants. Selected participants will be invited to send an abstract highlighting the key features and talking points of their presentation.

If you have any questions, you can contact us at mdenet@kcl.ac.uk.

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Key dates

Call launched	13 July 2023
Call close (expressions of interest)	15 Sept 2023 at 17h
Participant invitations:	20 Sept 2023
Profile videos or doc slide:	18 Oct 2023
Workshop:	31 Oct 2023