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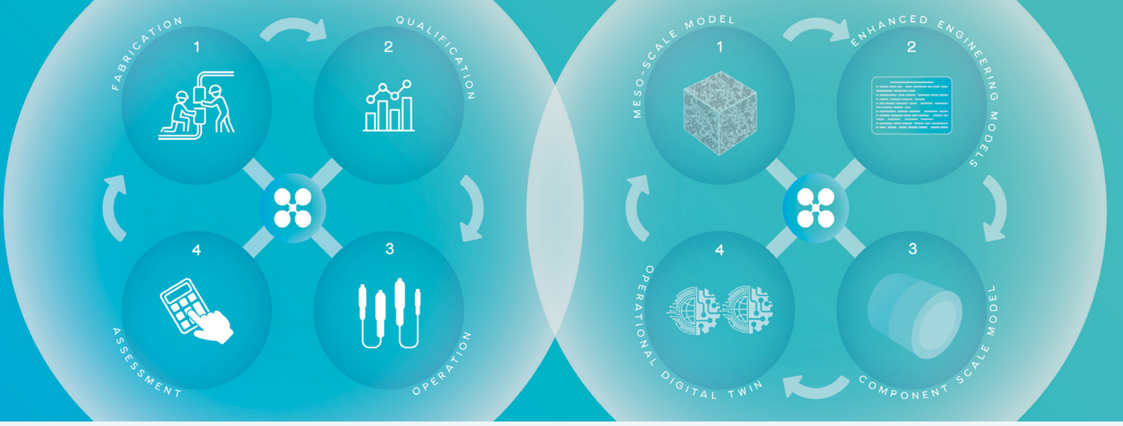
PROSPERITY PARTNERSHIP



SINDRI: Synergistic utilisation of INformatics and Data centRic Integrity engineering - 2023 Annual Report

Business Lead: EDF | University Lead: University of Bristol | Grant reference: EP/V038079/1

SUMMARY

The Synergistic utilisation of INformatics and Data centRic Integrity engineering (SINDRI) Prosperity Partnership is developing digital tools that will initiate a step-change in the nuclear industry's design and in-service assessments of materials and components. These tools will speed up the implementation of innovative designs and transform the way the industry conducts structural assessments. SINDRI will use advanced predictive materials models, underwritten by high fidelity experiments, together with model reduction methods, to translate manual processes to a virtual environment which enables the application of robust probabilistic-based assessments.

INTRODUCTION AND BACKGROUND

The nuclear industry faces substantial challenges in delivering cost effective technical advancements which will impact its contribution to a net zero carbon economy by 2050. The SINDRI project aims to develop open-source, digital tools that will accelerate construction and reduce OPEX in the nuclear industry. By building a comprehensive suite of software, the project aims to eliminate significant time-consuming and cumbersome human interventions enabling high throughput analysis which can accommodate next generation digital tools. SINDRI is a collaborative effort between academia and industry and supports several national initiatives such as the Advanced Modular Reactor Programme. A Prosperity Partnership is an excellent route to achieve the objectives of SINDRI as it brings together key expertise across science and engineering and provides a rapid route for testing and implementation within industry.

KEY TECHNICAL OBJECTIVES

- Quantify the effects of fabrication and in-service environment on materials microstructure and its evolution using high-fidelity experiments.
- Employ and develop microstructurally informed, multi-physics models to simulate fabrication and in-service behaviour of representative alloy systems.
- Implement data-driven methods and approaches such as model reduction, data assimilation, and uncertainty quantification to enable modelling activities to cross length scales.
- Provide a controlled and validated toolbox of approaches to the nuclear industry to underpin a robust probabilistic approach distinct from the current, expensive, and conservative deterministic methods.

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PROJECT ACHIEVEMENTS: OUTPUTS, OUTCOMES, AND IMPACT

At its midpoint, the SINDRI project has made significant progress, successfully completing key technical deliverables and trialling of technologies with industrial partners. A core focus is integrating numerical tools across length scales, realised through the development of the SINDRI Toolbox. This toolbox serves as a central hub for seamlessly incorporating diverse numerical tools and associated components. Below we highlight some project achievements on the toolbox and the tools and components that feed into it:

The SINDRI Toolbox

The SINDRI Toolbox aims to facilitate and showcase the advantages of employing a data-centric approach to structural integrity analysis. It will provide a secure and robust way of capturing and integrating “modules” developed within the SINDRI project. Importantly it will ensure that modules developed in isolation can integrate with each other. The Toolbox takes the form of a GitLab repository, with the goal to allow users to carry out the following tasks along a workflow (Fig 1):

- Entry into service predictions of critical component microstructure, e.g. welds.
- In-service degradation assessments on a material meso-scale.
- Probabilistic structural integrity assessments on a component scale.

The SINDRI Toolbox V0.1 has been released containing three modules:

1. Phase field module: for entry into service predictions.
2. EBSD to CPFE module: for in-service degradation predictions.
3. Welding Workbench module: For component scale structural assessments.

The first module enables users to apply phase-field methodologies to predict the microstructure that arises from welding processes. The second module enables users to use electron microscopy-based characterisation techniques to generate crystal plasticity based finite element (CPFE) models. These models can be used to understand the through life material properties on a meso-scale, accounting for grain size, texture and morphology. The third module enables users to rapidly generate macro-scale weld simulations. Following academic and industrial best practices and guidance, it can be used to obtain residual stress predictions in austenitic stainless and ferritic steel weldments. All the modules are built, tested, and containerised using open-source tools, enabling simplistic configuration, development, and deployment of the Toolbox (Fig 1). Regular developer meetings are held to facilitate knowledge exchange and training. These meetings also provide a platform for academia and industry to interact directly on technical issues, while keeping a close eye on the source code and incorporating new developments.

Surrogate Modelling: Bridging the Gap

The integrity of components in safety critical industries is a consequence of the mechanical properties and behaviour of the material from which they are fabricated. While SINDRI has developed high fidelity models of the behaviour of key materials within the nuclear industry as a function of their underlying mesostructure, the application of the models is practically limited to a very small volume of material – a consequence of their high computational demands. Extending the simulated properties of materials from the mesoscale to industry relevant volumes (and hence components) has been the main hurdle in the wide usage of such material models, not just in nuclear but in many other applications.

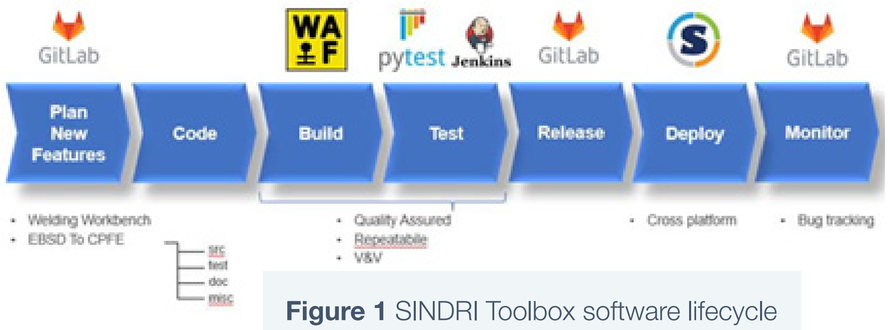


Figure 1 SINDRI Toolbox software lifecycle

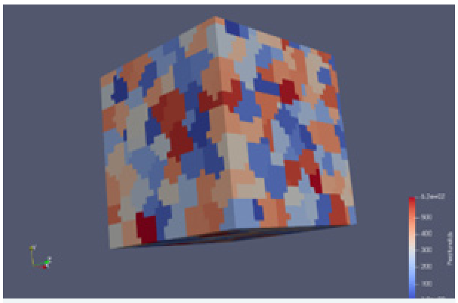


Figure 2 A Representative volume element of a material simulated by crystal plasticity finite element portraying only one combination of microstructure.

This barrier has raised further fundamental problems as the uncertainty associated with the large number of calibrating parameters governing the model are estimated using a limited number of experiments. This in turn limits the application of probabilistic methods to be built using the models to determine the underlying variability in material properties.

In SINDRI, we have addressed these problems through application of the concept of surrogate modelling to statistically bridge the gap between the properties estimated by a model of a small representative volume of material and that of a large structure, incorporating the variation of its microstructure. As a proof of concept, we have successfully applied polynomial chaos expansion to estimate the uncertainty of mechanical response of stainless steel 316L, a material widely used in the nuclear industry, through our crystal plasticity models as a result of change in the material grain size, morphology and texture.

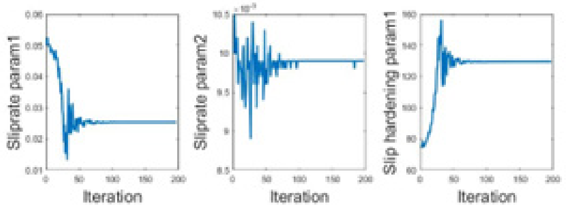


Figure 3 Calibration of parameters governing the crystal plasticity finite element model using surrogate modelling technique which can reduce the number of iterations significantly.

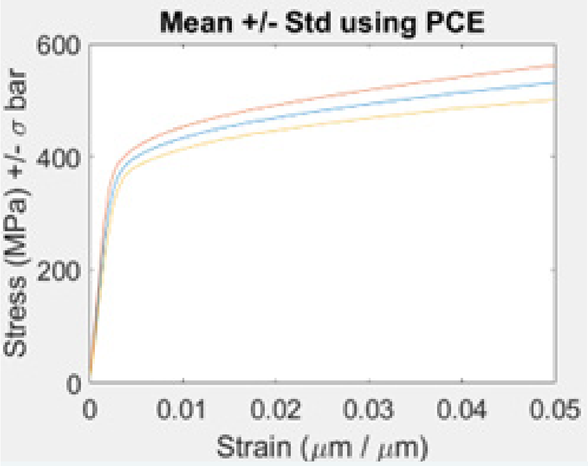


Figure 4 Predicted variation in the mechanical response of the material shown as mean and standard deviation as a function of variation in the texture of crystals forming the alloy using polynomial chaos expansion reduces the number of iterations significantly.

Multi-Phase Multi-Component Modelling of Solidification Microstructures

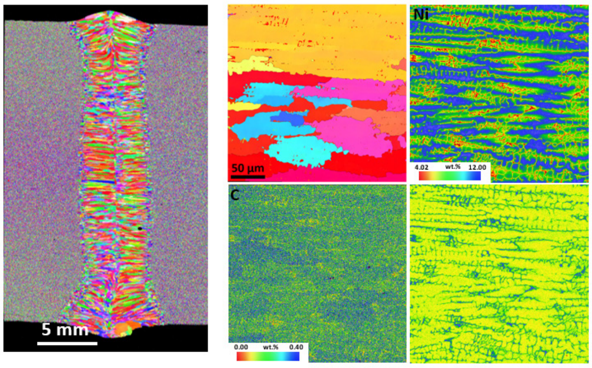


Figure 5 Columnar Grains (Dendrites) Observed Experimentally.

Solidification microstructure in metallic substrates largely determine its mechanical properties aniosotropy. The growth kinetics of dendrites within multi-component alloys is strongly influenced by the local composition ahead of the advancing solid-liquid interface as solute species are rejected. Additionally, fluid flow around, and through, the dendrites can act to re-distribute this rejected solute and perturb the growth of dendrites. In this work we used a CALPHAD-informed multi-component, multi-phase field framework, including conservation of momentum, mass, and energy to investigate the role of melt velocity fields in the re-distribution of solute and associated changes to dendritic growth morphologies.

This multi-component multi-phase field code is currently too computationally expensive for simulation of the full thickness of a weld in an industrially relevant component, and therefore work has continued on the lower-fidelity, single-component, multi-phase code through comparison with microstructural data.

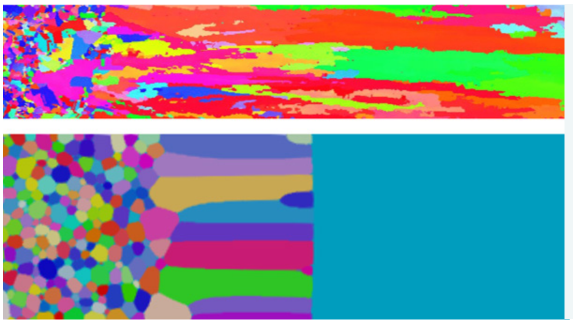


Figure 6 EBSD IPF-X

Microstructure-informed continuum modelling of weldments

Further refinement of the multiscale modelling approach for predicting the mechanical response of an electron beam weld in stainless steel 316L has allowed for an improvement in the mechanical response prediction in the weld metal. Fig 7 demonstrates this – it was achieved by performing a stricter convergence criterion of the representative volume elements and also by applying the exact weld process strains. This led to an improvement in the component scale stress predictions was achieved as seen in Fig 8.

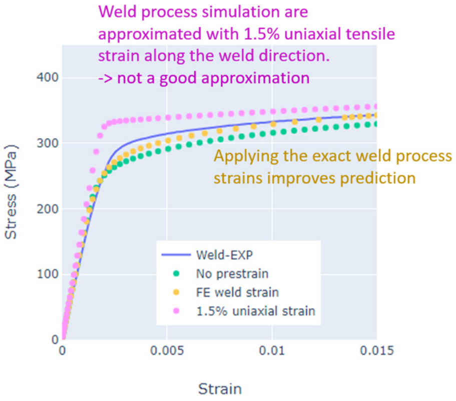
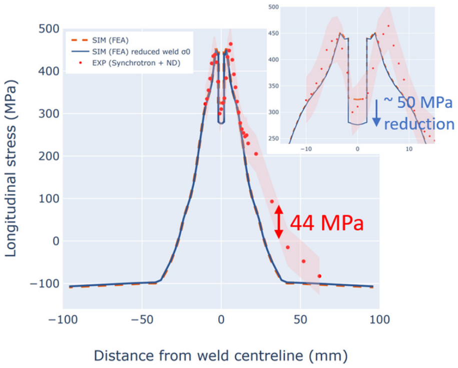


Figure 7 Stress-strain curves in the 316L weld metal as measured by experiment and modelled using different pre-strain conditions.

Figure 8 Longitudinal residual stress versus distance from the weld centreline at mid-thickness.



The next stage is looking at ferritic steels. This is a more challenging task as they undergo a solid-state phase transformation during welding which alters the deformation field and the mechanical properties of both the weld and the heat affected zone. Therefore, the microstructural development needs to be experimentally measured or modelled and then incorporated in our numerical model as a function of time and temparature.

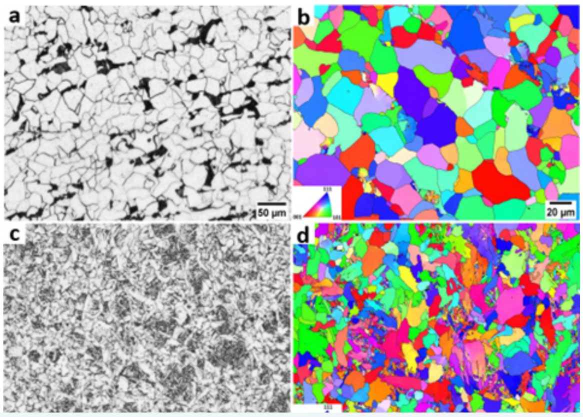


Figure 9 – (a) and (c) Light optical micrographs and (b) and (d) inverse pole figure (IPF)-Z direction maps from EBSD analysis showing the resulting microstructure of ferritic steel submerged arc welded submitted to heat treatment at 1200 oC for 10s followed by continuous cooling at (a-b) 0.2 oC/s and (c-d) 20 oC/s.

Development of a novel image analysis technique to determine the creep deformation and failure properties under multiaxial stress conditions

Creep deformation and damage is strongly dependent on the materials stress state, with a high stress triaxiality promoting more creep damage. Notched bar creep tests with a range of notch radii enable the relationship between stress triaxiality and creep strain to be determined (Fig 10). A novel optical image analysis technique has been developed to quantify the evolution of the notch acuity with time through measuring the notch throat minimum radius, a, and the notch radius, R, during a creep test (Fig 11). These results are being used to develop and validate numerical models to predict both creep deformation and damage under multiaxial stress conditions. These validated models can then be applied to components in plant.

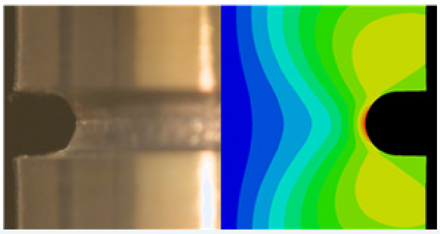


Figure 10 – Image of an axisymmetric 316H steel notched bar sample at 550 °C compared to finite element axial displacement contour plot.

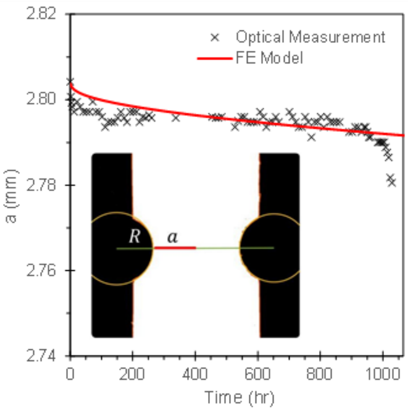


Figure 11 Reduction in sample notch throat radius with time from experimental image analysis and finite element (FE) model prediction.

ENGAGEMENT, DISSEMINATION AND AWARDS

The SINDRI team have been disseminating their work and engaging stakeholders at various events and conferences nationally and internationally. Highlights include:

- 2023 SINDRI Conference (UK) - An internal conference hosted by the project consisting of talks and presentations attended by 45 project members and researchers from connected projects.
- Regulator and Supply Chain Expert Panel: Regulation of Artificial Intelligence in Nuclear (UK) - Participants

- AI and Data Science Summit: The Role of Data Science in the Lifecycle of Critical Components (UK) - SINDRI co-hosted this industry-academia summit together with other related EPSRC projects. The summit consisted of talks, posters and a sandpit competition where teams developed solutions to future data science challenges. Held in collaboration with the Henry Royce and Alan Turing Institutes.

- Report on data-centric engineering approaches in nuclear (UK) – SINDRI produced a report detailing challenges and recommendations for the nuclear sector to adopt digital engineering practices. The report was based on SINDRI-hosted workshops and conversations with key players such as EDF, Rolls Royce, UKAEA, and others.
- Visit from the French Commission for Atomic Energy (CEA) – Expanded the international industrial links of the project with the leading European country in nuclear energy.

- British Science Week (UK) – Demonstrations and workshops by PDRA Maria Yankova.
- Project team presented at several national and International conferences including PVP (Atlanta USA), ESIA (Manchester UK), CSBMM (Brazil), The Advanced Materials Show (UK) and ICF (Atlanta USA).
- Australian Nuclear Science and Technology Organization (Australia) - Secondment and code deployment by Co-I Nicolo Grilli to further expand the international reach of the project impact.
- ElectroChem2023 Shreir prize (2023) awarded to PhD student James Rafferty (The University of Manchester) for best presentation.

TEAM DEVELOPMENTS

The SINDRI team has recruited positions in both academia and industry and the team is more balanced across experimentalists and the modelling community.

Dr Farhan Ashraf has joined as a PDRA at the University of Bristol and strengthens our numerical modelling activities. Dr Raheeg Ragab and Simon Lewis have joined as researchers in the Advanced Reactor & Structural Integrity R&D group at EDF and improve the translation of the modelling work into EDF. Through these appointments and growth in the team at EDF, our relationship and interactions between collaborators have grown stronger.