# EXCALIBUR



# SEAVEA: Software Environment for Actionable and VVUQ-enabled Exascale Applications

Presenter: Derek Groen Investigators: Peter Coveney, Serge Guillas

Bristol, 11-12 October 2023



UK Research and Innovation

UK Atomic Energy Authority

### **Project Overview**



We aim to develop a generic exascale toolkit to enable application users to make their models more robust and the results actionable through e.g.:

Argonne

ve the Children

- uncertainty quantification (aleatoric and epistemic)
- sensitivity analysis
- ensemble forecasting
- ensemble validation
- on-the-fly verification
- training and large-scale application of surrogate models.

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

August 2021 - October 2024

https://www.seavea-project.org







### **Current Project Status**

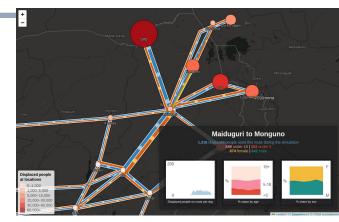
We have made our third SEAVEAtk release: <a href="https://www.seavea-project.org/seaveatk/">https://www.seavea-project.org/seaveatk/</a>

Several major research outputs:

- FabSim3 paper in CPC
- Sensitivity analysis with correlated parameters (preprint)
- Robust simulation dev for emergency response.
- Release of TIES 2.0 (CBMX)
- Flee forecasting collaboration with Save the Children

Events:

- More more hackathons!
- Tutorial sessions at home and abroad
- HPC Workshop at LRZ in Munich.
- <u>https://mms.computationalscience.nl</u>



https://williamlow.github.io/ABM/ABM nigeria update.html



Journal of Computational Science Volume 72, September 2023, 102107

Facilitating simulation development for global challenge response and anticipation in a timely way

Derek Groen 🙁 🖾 , Diana Suleimenova, Alireza Jahani, Yani Xue

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https://doi.org/10.1016/j.jocs.2023.102107 🛪



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Statistics > Methodology

[Submitted on 31 May 2023]

Sensitivity Analysis of High-Dimensional Models with Correlated Inputs

Juraj Kardos, Wouter Edeling, Diana Suleimenova, Derek Groen, Olaf Schenk



Computer Physics Communications Volume 283, February 2023, 108596

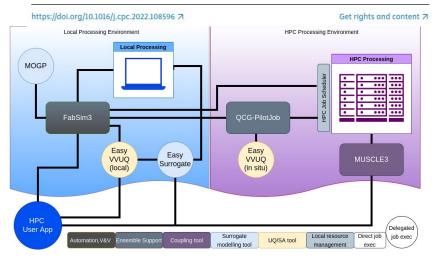


Feature article FabSim3: An automation toolkit for verified simulations using high performance computing \$\frac{1}{2}\$

<u>Derek Groen <sup>a d</sup> A</u> ⋈, <u>Hamid Arabnejad</u> <sup>a</sup>, <u>Diana Suleimenova</u><sup>a</sup>, <u>Wouter Edeling</u><sup>b</sup>, <u>Erwan Raffin</u><sup>c</sup>, <u>Yani Xue</u><sup>a</sup>, <u>Kevin Bronik</u><sup>d</sup>, <u>Nicolas Monnier</u><sup>c</sup>, <u>Peter V. Coveney</u><sup>d e f</sup>

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### **Strengths & Challenges**



- Strengths
  - Solid user uptake of SEAVEAtk across the board.
  - Good team of maintainers, with long-term interest.
  - Clear upticks in research and code outputs.
    - A lot of working papers going on as well.
    - Next SEAVEAtk release planned for December.
- Challenges
  - Technical: UQ and ensemble simulation beyond 100,000 cores / jobs.
    - Two horses: QCG-PilotJob & RADICAL Cybertools
  - People barrier: Looking for PhD student opportunities & recruitment challenges.
  - Funding barrier: Looking for VVUQ / simulation research opportunities.
    - SEAVEA ends October next year, no follow-up funding yet.



# Thank you



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