National centre for innovative software solutions in academic research

Information event
Open eScience Call 2023
Welcome to the information event

Open eScience Call 2023
Early Career & Spearhead Projects

“Empowering researchers through digitally enhanced research”

https://www.esciencecenter.nl/calls-for-proposals/open-escience-call-2023-oec-2023/
Program

- 13:00 Netherlands eScience Center introduction and purpose of calls
- 13:15 Current call for proposals
- 13:30 Netherlands eScience Center expertise
- 13:45 Software management plan
- 14:00 Break
- 14:15 SURF research infrastructure
- 14:30 Q&A session
- 15:30 END
What is the eScience Center?

“The eScience Center is a **research organization** the task to ensure that the Netherlands remains at the **forefront of international research** in applying **research software** to answer challenging, urgent **research questions**.

We fulfil this purpose by contributing to a robust national research community in which ultimately **all investigators in all disciplines** will be able to exploit **advanced digital technologies**.”

- national centre of expertise
- independent foundation (2012)
- NWO & SURF
- Research Software Engineers (RSEs)
- strategy 2021-2025: two ambitions
Which calls do we have?

**Open eScience Call**
- “Empowering researchers through digitally enhanced research”
- Information event 14 February

**Call for Sustainable Software**
- “Enhancing successful research software”
- Information event 21 February

*(we have more Calls, so subscribe!)*
How do we work?

- we **collaborate** with researchers in projects of varying size
- projects are driven by **research challenges** faced by project partners
- we offer **expertise (in-kind)**, not money (in-cash)
- we apply **state-of-the-art solutions** from computer science and digital infrastructure
- our research software, data and knowledge is **reusable & open**
- we encourage **software sustainability**, with all projects investing in **communities**
What are RSEs?

• specialized, high-end researchers (most have a PhD), who have
• a broad orientation + strong affinity with ICT, so that
• they understand both the research question and modern ICT solutions
  • (a) performing research focused on digital technologies and methodologies
  • (b) engineering software
• 70-80 RSEs are members of the eScience Center community
What is the objective of the OEC Call?

“This call for proposals supports state-of-the-art and innovative research that requires the development and application of advanced research software.

Each submitted proposal should address an urgent methodological research challenge that can count on broader support from the research community in which the applicants are active.

The call reflects the eScience Center’s strategy to advance the use of sustainable research software in academic research.”
What makes the OEC Call special?

• fully in-kind (unlike NWO or Horizon Europe)
• non-technological research question (unlike Sustainable Software Call)
• strong focus on workshops and impact
• simplified application procedure
Current CfP: Who can apply?

• ‘Lead Applicant’
  • Affiliated to a Dutch research performing organization
  • In possession of a PhD
  • Holds a
    • permanent contract or tenure track position (for Spearhead Projects)
    • contract for at least the duration of the requested project (for Early Career Projects)
  • Knowledge and experience in applying digital methodologies to research
  • Ensure a minimal personal commitment to the project work for half a day per week on average for the duration of the project.

Researchers who are involved in a project awarded under the eScience Center OEC 2021 or OEC 2022 Calls in the capacity of Lead Applicant (or ‘Principal Investigator’) are not allowed to submit as LA in this call.
## Current CfP: What can be applied for?

<table>
<thead>
<tr>
<th></th>
<th>Early Career Projects</th>
<th>Spearhead Projects</th>
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<tbody>
<tr>
<td>Requirements for LA</td>
<td>PhD, not more than 6 years ago</td>
<td>PhD</td>
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<tr>
<td></td>
<td>Contract for duration of project</td>
<td>Permanent contract or tenure track position</td>
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<td>Demonstrable experience in applying digital methodologies to research</td>
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<td>LA commitment of on average half a day per week for the duration of the project</td>
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<td>Software Management Plan with optional support letters</td>
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<tr>
<td>Conditions projects</td>
<td>Duration: 12-18 months</td>
<td>Duration: 24-30 months</td>
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<td></td>
<td>Support from eScience Center RSEs: 1.5 PYR</td>
<td>Support from eScience Center RSEs: 2.5 PYR</td>
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<td>Single LA, team members are not mandatory but encouraged</td>
<td>Single LA, team members required (at least one from a different Dutch research institute)</td>
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<td>No. of workshops: 1</td>
<td>No. of workshops: at least 2</td>
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<td>Max. workshop expenses: 15.000 EUR</td>
<td>Max. workshop expenses: 25.000 EUR</td>
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<td>A clearly defined research challenge from one of the following discipline areas: Life Sciences (LS) / Physical Sciences and Engineering (PSE) / Social Sciences and Humanities (SSH)</td>
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<td>Available projects</td>
<td>7 (2 each for PSE and LS; 3 for SSH)</td>
<td>4 (1 each for LS and SSH; 2 for PSE)</td>
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Current CfP: Workshops

OEC Early career projects
• The eScience Center will help applicants submit their workshop proposal to the Lorentz Center.
• The eScience Center will cover the costs for the organization (up to a maximum)

OEC Spearhead projects
• At least two substantial mandatory workshops
• LAs should negotiate the format and costs of the workshops with the eScience Center.
• The eScience Center will cover the costs for the organization (up to a maximum)

Workshops are focused, participatory events with the aim of creating or fostering a community of researchers, including (potential) users, around the digital technologies and research software produced within the project.
Steps in procedure

- Information event
- Project proposition
  - No other documents needed
  - Submission via ISAAC
  - Eligibility check
    - Match with eScience center expertise
    - Rules in “who can apply?”
  - Random selection of eligible Project Propositions
- Consultation sessions
  - Friendly advice from eScience Center employees on proposal
- Full proposal
  - Full Proposal document
    + Software Management plan
    + (Optional) Support letters
  - Submission via ISAAC
  - Eligibility check
  - Software and Data Health Check
  - Panel assessment
    - Domain experts
    - eScience experts
- Awarding
  - eScience Center Board
Current CfP: Timetable

- 14 February 2023: information event
- **16 March 2023, 14:00 CET**: deadline project proposition
- March-April 2023: eligibility check, selection and notification
- April-May 2023: consultation sessions
- **8 June 2023, 14:00 CET**: deadline full proposal + software management plan
- June 2023: eligibility check
- September-October 2023: panel assessment
- November-December 2023: applicants informed of final decision
eScience Center
Technological Competences
Our Technological expertise

- Artificial Intelligence
  - Machine Learning
  - Image Processing

- Analytics
  - Big Data Analytics
  - Text Analysis
  - Visualization

- Data processing
  - Databases
  - Real-time Data Analysis
  - Interoperability and Linked Data

- Computing
  - Exploiting Hardware Accelerators
  - High Performance Computing
  - Cloud Computing
  - Combining Simulations

Software quality

- Developing Workflow Technologies
- Improving Software Practices
- Advancing Software Sustainability
- Increasing Academic Impact
DeepRank

Scoring 3D protein-protein interaction models using deep learning

Interactions between biomolecules control all cellular processes. Understanding those interactions requires adding a three-dimensional structural dimension. Next to experimental structural biology techniques, this can be done by docking, a complementary and high-throughput computational method allowing to model complexes from their known components.

A challenge in docking is scoring – the identification of correct (near-native) models from a large pool of docked models – due to our still limited knowledge of interaction rules. We will tackle this challenge by training deep networks (dNNs) to learn complex interaction patterns from the huge amount of experimental data in the Protein Data Bank (a valuable source of information not yet fully exploited). Our innovative strategy is to treat this problem as a 3D image classification problem: The interfaces of docked models will be represented as 3D images and dNNs will be trained to classify whether they are near-native or not. Unlike other machine learning techniques, dNNs are now able to learn from millions of data without reaching a performance plateau quickly, which is computationally tractable by harvesting GPU and Hadoop technologies.

The resulting scoring function, DeepRank, will markedly enhance our capability to reliably model biomolecular complexes, assisting the scientific community to gain insights into macromolecular aspects of life. It will be implemented in our HADDOCK modeling platform and freely distributed through GitHub and eStep repositories, ensuring a wide dissemination. The impact will be broad since 3D image-based dNNs have applications in many other domains, such as medical diagnoses (MRI), cryo-electron microscopy and computer vision.
Research Software Directory

Show your research software to the world

The Research Software Directory is designed to show the impact research software has on research and society. We stimulate the reuse of research software and encourage proper citation of research software to ensure researchers and RSEs get credit for their work.

All software contributed to by the eScience Center is added to the Research Software Directory

https://research-software-directory.org/
Research Software Directory

• Finding software
• Making software accessible
• Quickly judge relevance and usage
• Indicating return on investment

All software contributed to by the eScience Center is added to the Research Software Directory

www.research-software.nl
Software findability (for humans)

What is the software for?

What problem does it solve?

For which research domain?

ESMValTool

The Earth System Model eValuation Tool is a community diagnostics and performance metrics tool for the evaluation of Earth System Models that allows for routine comparison of models and observations.

What ESMValTool can do for you:

- Facilitates the complex evaluation of ESMs and their simulations submitted to international Model intercomparison Projects (e.g., CMIP).
- Standardized model evaluation can be performed against observations, against other models or to compare different versions of the same model.
- The scope includes many diagnostics and performance metrics covering different aspects of the Earth System (e.g., climate, ocean, carbon cycle, chemistry, aerosols, sea ice, etc.) and their interactions.
- Well-established analysis: standard recipes reproduce specific sets of diagnostics or performance metrics that have demonstrated their importance in ESM evaluations in the peer-reviewed literature.
- High consistency: new diagnostics and more observational data can be easily added.
- Multilingual support: Python, R, Julia, ... other open-source languages are possible.
- OT (CMOR compliant): data from many different projects can be handled (CMIP simulations, analyses, CO2, COSMOS, etc.). Routines are provided to CMORize non-compliant data.

The Earth System Model Evaluation Tool (ESMValTool) is a community diagnostics and performance metrics tool for the evaluation of Earth System Models (ESMs) that allows for the routine comparison of single or multiple models, either against pre-established versions or against observations. The priority of the effort has been to target specific scientific themes focusing on selected Earth System variables, a range of process-oriented baselines and common to ESMs, such as coupled tropical climate variability, monsoons, Southern Ocean processes, continental dry areas and soil hydrology climate interactions as well as atmospheric CO2 budgets, troposphere and stratosphere ozone and tropospheric aerosols. The tool is being developed in such a way that additional analyses can easily be added. A set of standard recipes for each scientific topic reproduces specific sets of diagnostics or performance metrics that have demonstrated their importance in ESM evaluation in the peer-reviewed literature. The ESMValTool is a community effort open to both users and developers encouraging open exchange of diagnostic source code and evaluation results from the CMIP ensemble. The tool will facilitate and improve ESM evaluation beyond the stated level and sets of supporting such activities with the Coupled Model Intercomparison Project (CMIP) and at individual modeling centers. Ultimately, we envisage running the ESMValTool alongside the Earth System Grid Federation (ESGF) as part of a more routine evaluation of ESM model simulations while utilizing observations available in standard formats (e.g., NetCDF) provided by the users.
Academic and social context

Projects with ESMValTool

Papers, presentations, blogs, videos ...

Projects

People
Development activity & how to cite

mcfly

Helps you find a suitable neural network configuration for deep learning on time series.

How to get started

Development activity

Software citation
Software and Data Health checks

Part of the full proposal review

We check the accessibility and quality of existing data and software that the project builds on

Aims: prevent surprises, delay and disappointment after the project start
Infrastructural needs

- Infrastructural needs (if any), in terms of computing power, data storage capacity, fast data transfers, or otherwise
- Various solutions possible, including national infrastructure
- Facilities offered by SURF
Software Management Plans
How do we think about SMPs?
Practical guide to SMPs

- Core requirements for SMPs
- Different levels of management: **not all software is created equal!**
- **NOT** another bit of admin: software management leads to better science!

SMP core requirements

Figure 1. Software Management Plan requirements grouped by their focus.
How do SMPs look like?

Software Management Plan Template (Version 2023)

1. Please provide a brief description of your software, stating its purpose and intended user community.
   Some aspects to be considered:
   - What is the purpose of the software?
   - What is the software's intended user community?
   - Why are you developing this and not reusing existing software?

5. What measures will be taken during the project to ensure the long-term sustainability of the software developed in the project? (max. 300 words)
   Some examples include:
   - A researcher or RSE from a research institute is allocated to the project to co-develop the software during the project and help maintain it afterwards.
   - A community will co-develop the software and help maintain it afterwards.
   - Organizing workshops and hands-on user training to create or extend a community around the software.
   - The software will be developed as part of an overarching software suite used in other (research) projects.
   - A commercial partner interested in exploiting the software is included as co-applicant on the basis of a concrete in-cash or in-kind investment.

6. What measures will be taken to support the software after completion of the project? (max. 300 words)
   Some examples include:
   - The software is hosted by an institute and a user support desk is made available for a certain period.
   - The software is integrated into a research infrastructure based on a large community.
   - A commercial partner or spin-off will continue the support and development of the software.

7. What resources are needed to ensure the long-term usability and availability of the software, and how will these resources be funded or obtained? (max. 300 words)
   Some examples include:
   - Storage or compute infrastructure to host the software.
   - RSEs to maintain the software and support the community that uses it.
   - A user support desk.

8. Are there other measures that will be taken to promote the software's longevity? (max. 300 words)
   Some examples include:
   - Additional project proposals which will help to further develop the software.
   - The software is integrated into teaching in a course on the Bachelor or Master level.
   - Outreach through mainstream media such as newspaper articles, blogs, YouTube videos, tweets, etc.
We look forward to working with you!
“Empowering researchers across all disciplines through advanced research software”

Contact information

Programme Management
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e-science@nwo.nl

NWO ISAAC helpdesk
The ISAAC helpdesk is available from Monday to Friday from 10:00 to 17:00 hours at +31 (0)20 346 7179.

You can also send your questions to isaac.helpdesk@nwo.nl. You will receive a reply within two working days.