

1. General Project Information

Name Grant Holder & ORCID	Gerard Carrera i Cardona 0000-0001-6111-0594
Contributor name(s) (+ ORCID) & roles	Peter Dedecker 0000-0002-1882-2075 Florian L. R. Lucas 0000-0002-9561-5408
Project number & title	11Q4E24N "An attoscale stopped-flow device for the measurement of ensemble and single-molecule kinetics "
Funder(s) GrantID	FWO 11Q4E24N
Affiliation(s)	X KU Leuven <input type="checkbox"/> Universiteit Antwerpen <input type="checkbox"/> Universiteit Gent <input type="checkbox"/> Universiteit Hasselt <input type="checkbox"/> Vrije Universiteit Brussel <input type="checkbox"/> Other: Provide ROR identifier when possible: https://ror.org/05f950310
Please provide a short project description	The kinetics of chemical processes determine the basic functioning of living systems. Many techniques have been developed to measure chemical kinetics, but these have difficulties measuring under the conditions of very small volumes and low copy numbers often inherent to cells, where quantum effects or dynamic heterogeneity become important. In this project, we propose to develop a very original way of measuring chemical kinetics, by using nanopores to generate tiny mixing regions with volumes in the attoliter regime, which would in principle allow controlled measurements to be performed on sample amounts down to one single molecule. We will develop an initial implementation of this 'AttoSpark' technology, model and characterize its performance, and apply it to the measurement of both ensemble and single-molecule processes.

2. Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset Name	Description	New or Reused	Digital or Physical	ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR PHYSICAL DATA
				Digital Data Type	Digital Data Format	Digital Data Volume (MB, GB, TB)	Physical Volume
Microscopy data	Images of bilayers and pores	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input checked="" type="checkbox"/> Observational <input checked="" type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf <input type="checkbox"/> .txt <input type="checkbox"/> .rtf <input type="checkbox"/> .dwg <input type="checkbox"/> .tab <input type="checkbox"/> .gml <input checked="" type="checkbox"/> other: .tif <input type="checkbox"/> NA	<input type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input checked="" type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
Electrophysiology data	Electrical recordings obtained with the eONE or the Axon amplifiers	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input checked="" type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf <input type="checkbox"/> .txt <input type="checkbox"/> .rtf <input type="checkbox"/> .dwg <input type="checkbox"/> .tab <input type="checkbox"/> .gml	<input type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input checked="" type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input checked="" type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	

					<input checked="" type="checkbox"/> other: .abf <input type="checkbox"/> NA		
Spreadsheet data	Spreadsheet files of part lists, components, results and it's analysis, etc.	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input checked="" type="checkbox"/> Observational <input checked="" type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input checked="" type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf <input type="checkbox"/> .txt <input type="checkbox"/> .rtf <input type="checkbox"/> .dwg <input type="checkbox"/> .tab <input type="checkbox"/> .gml <input checked="" type="checkbox"/> other: .xls <input type="checkbox"/> NA	<input type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input checked="" type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
Notes	Qualitative notes summarizing the data collected on each experiment	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input checked="" type="checkbox"/> other: .rtf	<input checked="" type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
3D models	Files of 3d printed parts, created with fusion 360.	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input checked="" type="checkbox"/> other: .F3D	<input type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input checked="" type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB	

				<input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA		<input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
COMSOL Simulations	Simulation files of the COMSOL software, containing both files from HDB, and the Attospark	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input checked="" type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf <input type="checkbox"/> .txt <input type="checkbox"/> .rtf <input type="checkbox"/> .dwg <input type="checkbox"/> .tab <input type="checkbox"/> .gml <input checked="" type="checkbox"/> other: .mph / .mp hbin <input type="checkbox"/> NA	<input type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input checked="" type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
Scripts	Scripts written mainly in Python, Rust, IgorPro etc.	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf <input type="checkbox"/> .txt <input type="checkbox"/> .rtf <input type="checkbox"/> .dwg <input type="checkbox"/> .tab <input type="checkbox"/> .gml <input checked="" type="checkbox"/> other: .py,.rs, etc.	<input type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input checked="" type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	

					<input type="checkbox"/> NA		
If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type.				I am not reusing existing data.			
Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, please describe these issues further and refer to specific datasets or data types when appropriate.				<input type="checkbox"/> Yes, human subject data <input type="checkbox"/> Yes, animal data <input type="checkbox"/> Yes, dual use <input checked="" type="checkbox"/> No If yes, please describe:			
Will you process personal data? If so, briefly describe the kind of personal data you will use. Please refer to specific datasets or data types when appropriate. If available, add the reference to your file in your host institution's privacy register.				<input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes:			
Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, ...)? If so, please comment per dataset or data type where appropriate.				<input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes, please comment:			

<p>Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/Data transfer agreements, research collaboration agreements)?</p> <p>If so, please explain to what data they relate and what restrictions are in place.</p>	<p><input type="checkbox"/> Yes</p> <p><input checked="" type="checkbox"/> No</p> <p>If yes, please explain:</p>
<p>Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use?</p> <p>If so, please explain to what data they relate and which restrictions will be asserted.</p>	<p><input type="checkbox"/> Yes</p> <p><input checked="" type="checkbox"/> No</p> <p>If yes, please explain:</p>

3. Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep **data understandable and usable**, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, Codebook.tsv etc. where this information is recorded).

Experimental data will be saved in folders named with the day it was acquired with the following convention: YYYYMMDD. In each day there will be a folder for each experiment, named accordingly. Inside each experiment folder there will be a folder for the Electrophysiology data (AXON_DATA) and a folder with the Microscopy Data (NIKON_DATA). And inside of each folder, the corresponding raw data files. Also inside the experiment folder there will be a metadata.rtf file explaining the conditions of the experiment. An example of the structured data would be like this:

```
20240312
20240313
├── Experiment1
│   ├── NIKON_DATA
│   │   └── data.tif
│   ├── AXON_DATA
│   │   └── data.abf
│   └── metadata.rtf
```

In the physical lab notebook, each page is headed with the date in the same format, and each experiment subheaded with the name of the experiment.

<p>Will a metadata standard be used to make it easier to find and reuse the data?</p> <p>If so, please specify which metadata standard will be used. If not, please specify which metadata will be created to make the data easier to find and reuse.</p> <p><i>REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.</i></p>	<p><input type="checkbox"/> Yes <input checked="" type="checkbox"/> No</p> <p>If yes, please specify (where appropriate per dataset or data type) which metadata standard will be used:</p> <p>If no, please specify (where appropriate per dataset or data type) which metadata will be created: The metadata, stored in the folder of the experiment will contain a detailed explanation of the samples used in the experiment, and the conditions used in the experiment.</p>
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4. Data Storage & Back-up during the Research Project	
Where will the data be stored?	<p>The primary storage location for the data will be the researcher's external hard drives for the Microscopy data, the electrophysiology data, and the notes. 3D model files will be stored in the computer and synced with the Fusion360 cloud. The other data will be stored in the researcher's personal computer.</p>
How will the data be backed up?	<p>Project data will be backed up to the KU Leuven OneDrive account. Big data files will also be backed up on the researcher's personal external hard-drive on a monthly basis. 3D files are automatically backed up with the Fusion360 cloud. Scripts are backed up in a personal Github repository.</p>
Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely. If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.	<p><input checked="" type="checkbox"/> Yes <input type="checkbox"/> No</p> <p>If yes, please specify concisely: We do have a large amount of Hard drives available that we can use, github is free, and OneDrive is included.</p> <p>If no, please specify:</p>

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?	Only I (the researcher) have physical access to my personal laptop, which is also password protected. The external hard-drive is kept in a secure location at home. Github, Fusion360, COMSOL, Dropbox and OneDrive accounts are also password-protected with 2 factor authentication.
What are the expected costs for data storage and backup during the research project? How will these costs be covered?	No additional costs are required for data storage for this project.

5. Data Preservation after the end of the Research Project

Which data will be retained for at least five years (or longer, in agreement with other retention policies that are applicable) after the end of the project? In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).	<p>The "Spreadsheet data" will be retained for at least five years after the research period.</p> <p>The "Microscopy data", "Electrophysiology data" and "Notes" will not, in their original form, be retained for five years after the research period. Due to the large space that they occupy. Modified parts of this files will be retained for at least five years after the research period.</p> <p>The "3D models" will be retained for at least five years after the research period.</p> <p>The "COMSOL Simulations" will be retained for at least five years after the research period.</p> <p>The "Scripts" will be retained for at least five years after the research period.</p>
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<p>Where will these data be archived (stored and curated for the long-term)?</p>	<p>The "Spreadsheet data" and "COMSOL Simulations" will, by the end of the research period, be kept in an external hard drive.</p> <p>Although the "Microscopy data", "Electrophysiology data" and "Notes" will not necessarily be retained for five years after the research period, the findings that they contain will be preserved long-term through publication as research articles and .</p> <p>For the "3D models" and "Scripts" will, by the end of the research project, be kept stored in the repositories.</p>
<p>What are the expected costs for data preservation during the expected retention period? How will these costs be covered?</p>	<p>There are no costs expected for the long-time preservation of the data.</p>

6. Data Sharing and Reuse

<p>Will the data (or part of the data) be made available for reuse after/during the project? Please explain per dataset or data type which data will be made available.</p> <p><i>NOTE THAT 'AVAILABLE' DOES NOT NECESSARILY MEAN THAT THE DATA SET BECOMES OPENLY AVAILABLE, CONDITIONS FOR ACCESS AND USE MAY APPLY. AVAILABILITY IN THIS QUESTION THUS ENTAILS BOTH OPEN & RESTRICTED ACCESS. FOR MORE INFORMATION: https://wiki.surfnet.nl/display/standards/info-eu-repo/#infoeu-repo-accessrights</i></p>	<p><input checked="" type="checkbox"/> Yes, in an Open Access repository</p> <p><input type="checkbox"/> Yes, in a restricted access repository (after approval, institutional access only, ...)</p> <p><input type="checkbox"/> No (closed access)</p> <p><input type="checkbox"/> Other, please specify:</p>
<p>If access is restricted, please specify who will be able to access the data and under what conditions.</p>	
<p>Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)? Please explain per dataset or data type where appropriate.</p>	<p><input type="checkbox"/> Yes, privacy aspects</p> <p><input type="checkbox"/> Yes, intellectual property rights</p> <p><input type="checkbox"/> Yes, ethical aspects</p> <p><input type="checkbox"/> Yes, aspects of dual use</p> <p><input type="checkbox"/> Yes, other</p> <p><input checked="" type="checkbox"/> No</p> <p>If yes, please specify:</p>
<p>Where will the data be made available? If already known, please provide a repository per dataset or data type.</p>	<p>The data will be made available in Gitlab.</p>
<p>When will the data be made available?</p>	<p>Upon publication of research results, or by the end of the research period (whichever happens sooner).</p>
<p>Which data usage licenses are you going to provide? If none, please explain why.</p>	<p>"3D models" and "Scripts" will be made available under a Creative Commons Attribution License (CC-BY 4.0), where the data creation is jointly credited to myself, my collaborators and the KU Leuven.</p>

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, please provide it here.	<input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes:
What are the expected costs for data sharing? How will these costs be covered?	There are no costs expected for the sharing of the data.

7. Responsibilities

Who will manage data documentation and metadata during the research project?	Gerard Carrera i Cardona (the researcher)
Who will manage data storage and backup during the research project?	Gerard Carrera i Cardona (the researcher)
Who will manage data preservation and sharing?	Gerard Carrera i Cardona (the researcher)
Who will update and implement this DMP?	Gerard Carrera i Cardona (the researcher)