POLYTECHNIQUE MONTRÉAL
UNIVERSITÉ D'INGÉNIERIE

July 17, 2023

Natural Resources Canada

Re: Submission of a NSERC's Alliance grant application

To the selection committee,

Please find enclosed an application for a NSERC's Alliance grant related to the Small Modular Reactor (SMR) opportunity. This application is tilted "Small modular reactors: Characterization of fuel and multi-year simulation of operation".

Truly yours,

Alain Hébert
full professor

Natural Sciences and Engineering Research Council of Canada
Conseil de recherches en sciences naturelles et en génie du Canada

FORM 101
Application for a Grant
PART I

Institutional Identifier	
System-ID (for NSERC use only)	561580003
Date	2023/08/10

Family name of applicant	Given name	Initial(s) of all given names	Personal identification no. (PIN)
Hébert	Alain	A	**Valid** 13665

Department	Institution that will administer the grant
Génie mécanique	École Polytechnique de Montréal

Language of application: [X] English [ ] French

What is the proposed cost-sharing ratio for this application? 50%

Type of grant applied for
Alliance Grants

Title of proposal
Small modular reactors: Characterization of fuel and multi-year simulation of operation

Provide a maximum of 10 key words that describe this proposal. Use commas to separate them.
nuclear reactor physics, deterministic lattice calculation, solution of the Boltzmann equation, small modular reactors, multi-year scenario simulation, fuel management and reprocessing, Dragon5 and Donjon5 simulation codes, high performance computing, UML user class model, multi layer perceptrons

Research subject code(s)		Area of application code(s)	
Primary	Secondary	Primary	Secondary
2401	2955	302	300

CERTIFICATION/REQUIREMENTS

If this proposal involves any of the following, check the box(es) and submit the protocol to the university or college's certification committee.

Research involving : [ ] Humans [ ] Human pluripotent stem cells [ ] Animals [ ] Biohazards

Indicate if any phase of the proposed research takes place outdoors and if you answered YES to a), b), c) or d), you must complete and attach Appendix A. See instructions for the Environmental Information Form. [X] NO [ ] YES

TOTAL AMOUNT REQUESTED FROM NSERC

Year 1	Year 2	Year 3	Year 4	Year 5
50,000	50,000	50,000	50,000	0

SIGNATURES (Refer to instructions "What do signatures mean?")

It is agreed that the general conditions governing grants as outlined in the NSERC *Program Guide for Professors* apply to any grant made pursuant to this application and are hereby accepted by the applicant and the applicant's employing institution.

Applicant

Head of department

Applicant's department, institution, tel. and fax nos., and e-mail

Génie mécanique
École Polytechnique de Montréal
Tel.: (514) 5143404711 ext. 4519
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alain.hebert@polymtl.ca

Dean of faculty

President of institution (or representative)

Personal identification no. (PIN)	Family name of applicant
Valid 13665	Hébert

CERTIFICATION/REQUIREMENTS

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Research involving :

Humans	Human pluripotent stem cells	Animals	Biohazards
[X] No [ ] Yes	[X] No [ ] Yes	[X] No [ ] Yes	[X] No [ ] Yes

Indicate if any phase of the proposed research takes place outdoors and if you answered YES to a), b), c) or d), you must complete and attach Appendix A. See instructions for the Environmental Information Form.

[X] No [ ] Yes

If "No", no further action required.

a) Will any phase of the proposed research take place on federal lands in Canada, other than lands under the administration and control of the Commissioner of Yukon, the Territories or Nunavut, as interpreted in section 2 of the Impact Assessment Act (IAA)? [ ] No [ ] Yes

b) Will any phase of the proposed research take place in a country other than Canada? [ ] No [ ] Yes

c) Will the grant permit a designated project (listed in the Physical Activities Regulations) to be carried out in whole or in part? [ ] No [ ] Yes

d) Will any phase of the proposed research activities depend on a designated project (listed in the Physical Activities Regulations) being led and carried out by an organization other than NSERC? [ ] No [ ] Yes

Personal identification no. (PIN)	Family name of applicant
Valid 13665	Hébert

CO-APPLICANTS

I have read the statement "What do signatures on the application mean?" in the accompanying instructions and agree to it.

PIN, family name and initial(s)	Organization	Signature
17913, Marleau, GCR	École Polytechnique de Montréal	

Personal identification no. (PIN)	Family name of applicant
Valid 13665	Hébert

Before completing this section, read the instructions for the definition of collaborators in the Eligibility Criteria section of the Program Guide for Professors.

COLLABORATORS

PIN, family name and initial(s)	Organization / Department
Doligez, X.	Université Grenoble Alpes,
Bidaud, A.	Université Grenoble Alpes,

Personal identification no. (PIN)	Family name of applicant
Valid 13665	Hébert

SUMMARY OF PROPOSAL FOR PUBLIC RELEASE (Use plain language.)
This plain language summary will be available to the public if your proposal is funded. Although it is not mandatory, you may choose to include your business telephone number and/or your e-mail address to facilitate contact with the public and the media about your research.

Business telephone no. (optional): 1 (514) 3404711 Ext. 4519
E-mail address (optional): alain.hebert@polymtl.ca

Nuclear reactor technologies are very serious options for energy production with low greenhouse gas (GHG) emissions and a reduced dependence on fossil fuels in the long term. Nuclear energy is characterized by extremely low lifetime GHG emission and very high-capacity factor, especially when compared to other low-emission energy sources. The future of nuclear energy is, in part, related to the successful design of innovative reactor technologies that use fuel efficiently and minimize radioactive waste. Canada's Small Modular Reactor (SMR) Action Plan is devoted to the development, demonstration, and deployment of SMRs for multiple applications at home and abroad. This research proposal focuses on the simulation of four innovative types of SMR for the characterisation of the fuel and waste using multi-year simulation of operation and storage:
(1) The BWXR-300 reactor from Aecon and GE Hitachi. The BWRX-300 is a 300 MWe Small Modular Reactor (SMR) design based on the boiling water reactor (BWR) concept. It features natural circulation with passive safety systems.
(2) The MMR-5 and MMR-10 HTGR concept. High-temperature gas reactors (HTGR) with fully ceramic micro- encapsulated (FCM) fuel that provides inherent reactor safety by being an ultimately safe fuel. TRISO particles, that maintain the radioactive byproducts of fission within a layered ceramic coating encased in a dense silicon carbide matrix.
(3) The ARC-100 concept. A modest scale up version of the successfully operated EBR-II, a 100-MWe sodium fast reactor (SFR) featuring sodium coolant and metal fuel assemblies. Two specific types of fuel are investigated: enriched uranium and reprocessed mixed metal fuel.
(4) The Stable Salt reactor concept from Moltex Clean Energy. The molten salt reactor (MSR) is a fast reactor that uses recycled nuclear waste as fuel. This is a class of nuclear fission reactor in which the primary nuclear reactor coolant and the fuel are combined into a molten salt mixture.

Other Language Version of Summary (optional).

Les technologies de réacteurs nucléaires sont des options sérieuses pour la production d'énergie avec de faibles émissions de gaz à effet de serre (GES) et avec une dépendance réduite aux combustibles fossiles à long terme. L'énergie nucléaire se caractérise par des émissions de GES très faibles et un facteur de capacité élevé. L'avenir de l'énergie nucléaire est lié à la conception de technologies de réacteurs innovantes qui utilisent efficacement le combustible et minimisent les déchets radioactifs. Le plan d'action du Canada pour les petits réacteurs modulaires (PRM) est consacré au développement et au déploiement de PRM pour de multiples applications au pays et à l'étranger. Ce projet de recherche porte sur la simulation de PRM innovants pour la caractérisation du combustible et des déchets par simulation pluriannuelle d'exploitation et de stockage :
(1) Le réacteur BWXR-300 d'Aecon et GE Hitachi. Le BWRX-300 est une conception de petit réacteur modulaire de 300 MWe basée sur le concept de réacteur à eau bouillante (BWR). Il dispose d'une circulation naturelle avec des systèmes de sécurité passive.
(2) Le concept HTGR MMR-5 et MMR-10. Réacteurs à gaz à haute température (HTGR) avec combustible micro-encapsulé entièrement en céramique (FCM) qui assure la sécurité inhérente du réacteur en étant un combustible intrinsèquement sûr. Utilisation de particules TRISO, qui maintiennent les sous-produits radioactifs de la fission dans un revêtement céramique et dans une matrice dense de carbure de silicium.
(3) Le concept ARC-100, un réacteur rapide au sodium (SFR) de 100 MWe doté d'un caloporteur au sodium. Deux types de combustibles spécifiques sont étudiés : l'uranium enrichi et les combustibles mixtes métalliques.
(4) Le concept de réacteur "Stable Salt" de Moltex Clean Energy. Le réacteur à sels fondus (MSR) est un réacteur rapide qui utilise des déchets nucléaires recyclés comme combustible. Il s'agit d'une classe de réacteurs à fission nucléaire dans lesquels le réfrigérant primaire du réacteur nucléaire et le combustible sont combinés en un mélange de sels fondus.

A. Background and expected outcomes

- Outline the goals of the partnership and explain the potential outcomes and impacts.
- Describe the importance of the topic to Canada and how the expected outcomes will benefit Canada.
- Explain the new concepts or directions needed to address the topic and how this research will fill knowledge gaps related to developing new and innovative policies, standards, products, services, processes or technologies in Canada. Position the proposed project relative to other efforts by the researchers and partner organizations and to any related research.
- Outline efforts the partner organizations will invest following the project's completion to advance the results in Canada.

Nuclear reactor technologies are very serious options for energy production with low greenhouse gas (GHG) emissions and a reduced dependence on fossil fuels in the long term. Nuclear energy is characterized by extremely low lifetime GHG emission and very high-capacity factor, especially when compared to other low-emission energy sources. The future of nuclear energy is, in part, related to the successful design of innovative reactor technologies that use fuel efficiently and minimize radioactive waste. Canada's Small Modular Reactor (SMR) Action Plan is devoted to the development, demonstration, and deployment of SMRs for multiple applications at home and abroad. This research proposal focuses on the simulation of four innovative types of SMR for the characterization of the fuel and waste using a multi-year simulation of operation and storage. Our proposal focuses on reactor physics tools support. More specifically, we propose to provide full support for (1) cross section evaluation processing based on the NJOY software, (MacFarlane, et al., 2010) (2) lattice calculations based on the Dragon5 software (Marleau, et al., 2023), (3) full-core simulation, including simplified thermal hydraulics, based on the Donjon5 (Hébert, et al., 2013) software, and (4) very long-term scenario simulations based on the CLASS software (Mouginot, et al., 2014).

Each SMR design is different and new tools need to be developed for each reactor concept. The biggest mistake would be to base these new tools on foreign intellectual property without full access by Canadian partner organizations (aka stakeholders) who need more than access to executable objects and prebuilt binary files. They should own and understand the internal coding of each Industrial Standard Toolset (IST) tool, the same way as the CANDU's Owner Group (COG) has access to the internal coding of their codes. This is the only way stakeholders can provide full support over decades of operation. SMRs require new types of fuel, different from the natural UOX bundles currently used in *Canada Deuterium Uranium* (CANDU) reactors. The optimization of fuel management for a single fleet design is possible at the computational scheme level. However, we need a more global strategy where the used fuel from a specific design is reprocessed and used in another reactor design. This type of optimization is only possible with scenario simulators like those we propose to develop. Canada's supply chain is well positioned to capture value. Supply chain goes from mining, fuel packaging for use in various designs, reprocessing and waste management in case reprocessing is not possible. The optimization at a more global level for the supply chain, that we propose, is both technically and economically desirable.

A first CNSC-sponsored Alliance grant was obtained in 2023 to focus on nuclear material accountancy produced by small modular reactors. It became clear that further R&D is required to support more SMR concepts, including the BWXR-300 reactor operated by Ontario Power Generation, and to study very long-term supply chain management issues related to the operation of multiple fleets of SMRs. These additional needs are motivating this new application. This project is a low-cost, high-benefit proposal. The funding is used only for graduate R&D related to M.Sc.A. and Ph.D. projects. All the R&D work is computer related and achieved on student laptops, local servers, and central processing units (CPU) located at the Digital Research Alliance of Canada.

We will focus on the adaptation of the Dragon5 and Donjon5 computer codes and to the design of computational scheme prototypes dedicated to these needs.

Stakeholders will be involved at each step of this project. They will provide use cases and specification requirements for the computational scheme prototypes related to the selected SMR concepts. Polytechnique Montreal will provide software components and training to the stakeholders upon request. Our contribution will provide full access to the nuclear reactor physics models underlying the SMRs, not only black box tools, as generally provided by the SMR vendors.

Partnership

- List all partner organizations expected to play a key role in the activities or to make cash and/or in-kind contributions.
- Describe the core activity of the partner organizations and their experience related to the research project, such as any efforts to date that the partner organizations have invested toward addressing this problem, the need for this research project and how the topic is relevant and aligned with the partner organizations' activities.
- Explain how each partner organization will be actively involved (through cash and/or in-kind contributions) in co-designing and implementing the research program. Describe the value added through in-kind contributions and how these are important to realizing the project's intended outcomes.
- Outline each partner organization's strategy and capacity to translate the research results into practical application to achieve the desired outcomes and impacts, including any planned knowledge translation activities and integration of the research results into its operations.

Today, stakeholders involved in SMR deployment are operators (Bruce Power, OPG and NB Power), consulting engineering companies (SNC-Lavalin, Kinectrics and Worley Parson), and designers of SMR concepts (GE-Hitachi and Aecom for BWRs, X-Energy for HTGRs, ARC nuclear for SFRs and Moltex Clean Energy for Molten Salt Reactors). The deployment of SMRs in Canada will be similar to the deployment of CANDU reactors decades ago but will provide more flexibility in supply chains. Success of CANDU deployment was possible because Canadian stakeholders (AECL and Ontario Hydro at that time) own the intellectual property of the computational schemes, design and operation tools specific to the CANDU technology. Today, these tools are known as IST and are used by stakeholders of the COG Alliance.

The research team at the *Institut de Génie Nucléaire* (IGN) will collaborate with many actors related to code distribution, reactor physics in general and SMR specialists in particular:

1. We already are in relation with the Nuclear Data Bank (NDB) of the Organisation for Economic Co-operation and Development (OECD) so as to integrate a new version 5.1.0 of Dragon5 and Donjon5 in their GetLab platform and to distribute these codes across the world.
2. We already are in relation with three consulting firms (Worley Parson, Kinectrics and SNC-Lavalin) so as to provide support and to adapt Dragon5 and Donjon5 for CANDU reactors. We plan to extend this support to SMRs.
3. We plan to contact the vendors of two of the SMR concepts selected in this Alliance proposal, namely the BWXR-300 reactor from Aecon and GE Hitachi and the Stable Salt reactor concept from Moltex Clean Energy, so as to gather reactor characteristics required for our simulations.

In the past, we collaborated with industrial organizations such as national laboratories (Atomic Energy of Canada Limited – AECL, Commissariat l'Énergie Atomique – CEA, Idaho National Laboratory – INL), industries (COG, Framatome, Électricité de France) and safety organizations (Institut de Radioprotection et de Sûreté Nucléaire – IRSN). All our graduate students are involved in the use and/or development of the DRAGON and DONJON codes, bringing this knowledge towards the industry.

Stakeholders are developing *computational schemes* dedicated to each reactor concept (CANDU or specific SMR concepts) using *software components* as building blocks. The role of Polytechnique Montréal is to provide these software components as Dragon5 or Donjon5 modules, to provide a Python scripting environment enabling the development of computational schemes and to provide support. Once available, the computational schemes are used by design teams to create a specific reactor concept, to perform nuclear safety assessment studies and to later develop its operating software. The software components provided by Polytechnique Montréal contain the basic reactor physics models required by the stakeholders under a GNU Lesser General Public License (LGPL), compatible with the non-disclosure agreements (NDA) required by the stakeholders to develop *production tools*. Moreover, using software components provided by Dragon5 and Donjon5 is the only option that guarantees a Canadian content for this basic software. This is the reason why the COG selected Dragon5 and Donjon5 as basic software components over the 2030-2060 timeframe. We promote the use of the same software components for SMR applications.

B. Proposal

- Outline the research objectives. Detail the resources and activities needed to achieve the anticipated results.
- Indicate approximate timelines for the activities to lead to milestones and deliverables using a Gantt chart, table or diagram.
- Explain how sex, gender and diversity have been considered in the research design, if applicable.
- Identify the indicators and methods for monitoring progress during the project and for assessing the outcomes. You may include a chart or table.

This research proposal is related to the implementation of computational schemes for different SMR concepts using deterministic solutions of the Boltzmann transport equation (BTE) or diffusion equation. Such solutions are orders of magnitude faster to obtain than stochastic solutions based on the Monte Carlo method. They make possible *scenario simulations* of the supply chain over decades or centuries of operations.

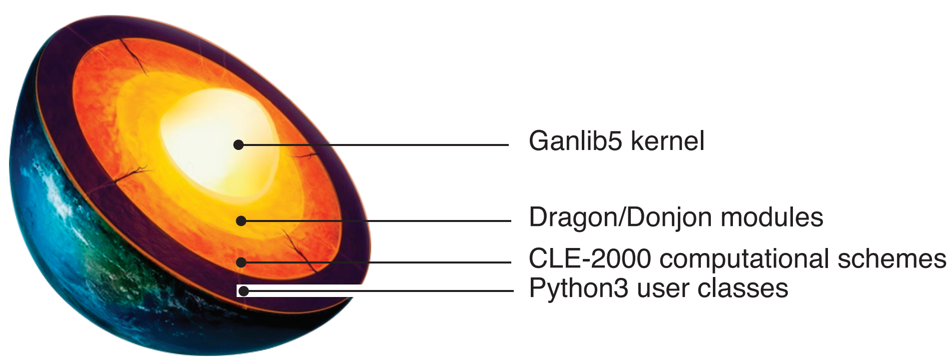

Fig. 1 Dragon5/Donjon5 architecture

The Dragon5/Donjon5 software is a kernel-based architecture, as depicted in Fig. 1. The Ganlib5 kernel (layer 1) is a C language implementation of the data structures and of the CLE-2000 supervisor. (Hébert, et al., 2022) Dragon/Donjon modules at layer 2 are independent building blocks in charge of performing elementary reactor physics duties such as performing a resonance self-shielding calculation, solving the BTE, solving the Bateman equations or building a multiparameter cross-section database for Donjon5. SMR support requires modifications at layer 2 and developments at the computational schemes and Python class layers. Python3 user classes can be developed using the PyGan extension classes as proposed in the

V5-PyKit prototype (Hébert, 2022). Production engineers are expected to be experts of the Python user class layer.

R&D at Polytechnique Montréal is related to four innovative types of SMR: (1) The BWXR-300 reactor from Aecon and GE Hitachi, (2) the MMR-5 and MMR-10 HTGR concept, (3) the ARC-100 concept, and (4) the Stable Salt reactor concept from Moltex Clean Energy. Types (2) and (3) are already investigated in the scope of a CNSC-sponsored Alliance grant. This research proposal will therefore focus on remaining types (1) and (4). However, all four types will be considered in the global simulation of subproject B.5.

Small modular reactors (SMR) feature unusual fuel compositions (e.g. plutonium, enriched uranium, reprocessed spent fuel), new physical fuel forms (hexagonal lattices, molten salts, TRISO particles, etc.) and different neutron energies in the core (fast spectra in ARC and some molten salt reactors). As a consequence of these differences, SMR nuclear material accountancy for spent fuel is expected to be very different from Canada Deuterium Uranium (CANDU) reactors. The proposed research proposal consists in extending and applying Dragon5 and Donjon5 to new reactor physics applications specifically those related to SMR. The combined benefits of this research will enable the optimization of the SMR deployment so as to minimize radiological risks, to reduce proliferation issues, to evaluate reprocessing capabilities and to better understand the outcome of an accident.

Better support of SMRs requires advances on selected subjects, identified as B.1 to B.6. A Gantt diagram is presented in Fig. 2 for a 36-months R&D plan. Deliverables are of two types: (1) Commits of SMR-specific code extensions in Dragon5 and Donjon5, and (2) technical reports, conference papers, articles and thesis defended according to the rules of Polytechnique Montréal. Extensions are committed in a continuous integration process. Publications are submitted for review after completion of each successful contribution.

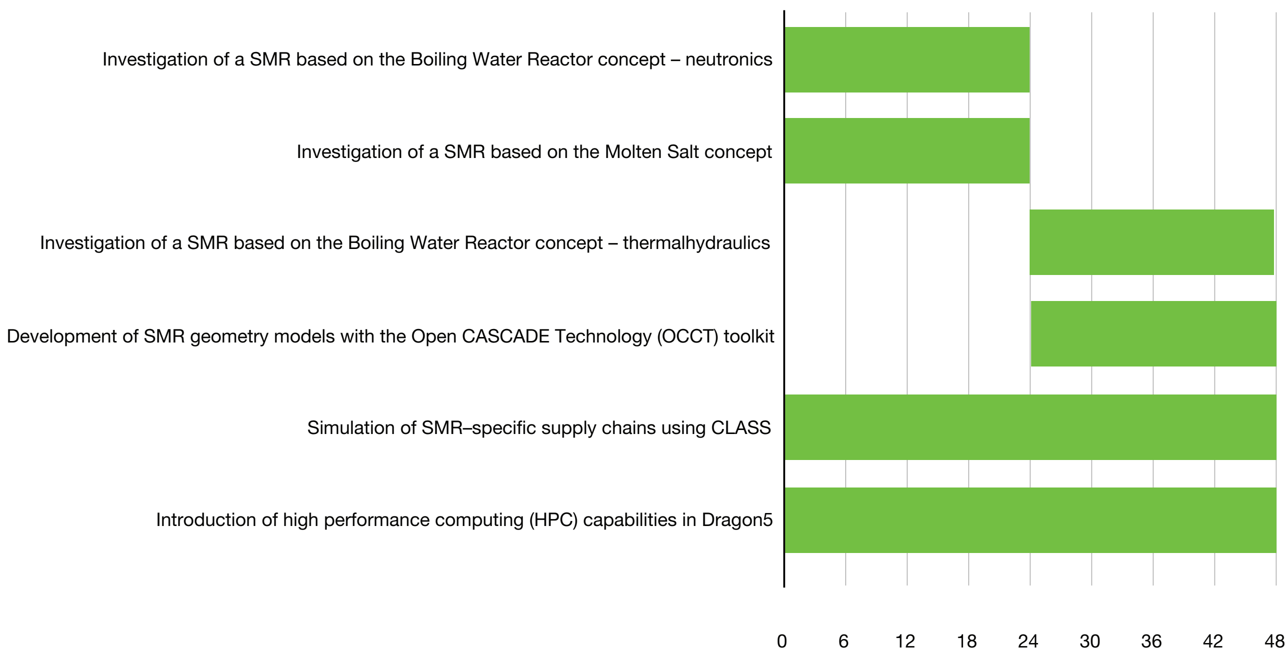

Fig. 2 Gantt diagram

The metrics to monitor progress throughout the project are based on the standard evaluation by pairs. External reviews are the best measure to determine if the research is on track.

Sex, gender and diversity are not considered in this research design and are not relevant to the study and optimization of material and fuel supply in the nuclear industry.

B.1 Investigation of a SMR based on the Boiling Water Reactor concept – neutronics (M.Sc.A.)

We will investigate the BWXR-300 reactor from Aecon/GE Hitachi. The BWRX-300 is a 300 MWe Small Modular Reactor (SMR) design based on the boiling water reactor (BWR) concept. It features natural circulation with passive safety systems. The subject of subprojects B.1 and B.2 is a contribution to the adaptation of Dragon5 and Donjon5 and to the development of Open-Source neutron calculation schemes adapted to this reactor concept. Aecon and GE-Hitachi already have neutronics and thermalhydraulic codes for the BWX-300 reactor, but these vendors put restrictions on their access (such as providing only binary executables of the codes to operators). Dragon5 and Donjon5 computational schemes will provide full access to the Fortran coding and to the reactor physics models behind the codes. Dragon5 code benchmarking will be based on detailed comparison with depleting SERPENT2 reference calculations, as these latter are highly reliable. Donjon5 code benchmarking will be addressed in subproject B.2.

For the neutronics perspective, BWR assemblies are more complex to model than those of pressurized water reactors (PWR) already supported by Dragon5. Tracking of three-level Cartesian geometries is currently missing in the SYBILT: and NXT: module of Dragon5. Only two-level geometries are supported. Such a three-level geometry is depicted in Fig. 3.

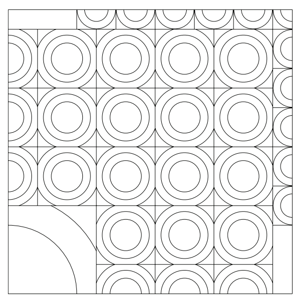

Fig. 3 Example of a three-level geometry in Dragon5

The proposed R&D approach in subproject B.1 is following:

1. Adapt Levon Ghasabyan's single-level PWR calculation schemes to the calculation of BWR assemblies
2. Study the benchmark proposed by H. Okuno *et al.* for BWR cells and assemblies. (Okuno, et al., 2002)
3. Perform SERPENT2 calculations in depleting Monte Carlo approximation.
4. Perform a deterministic (V5-PyKit) vs Monte Carlo (SERPENT2) comparison using Python3 scripts

B.2 Investigation of a SMR based on the Boiling Water Reactor concept – thermalhydraulics (M.Sc.A.)

BWR designs feature direct steam cycles between the reactor core and the turbine. The primary flow regime in a BWR is known as two-phase flow, as it involves the simultaneous presence of liquid water and steam. The two-phase flow regime can be further classified into two main patterns:

1. Subcooled Boiling: In this regime, the coolant flow is predominantly liquid, and boiling is limited. The coolant remains below its saturation temperature and is in a subcooled state. However, localized boiling can occur near the fuel rods due to the high heat generation. This regime is observed in regions of lower power density within the core.
2. Nucleate Boiling: As the coolant flows through regions of higher power density, it absorbs more heat and approaches or reaches its saturation temperature. Nucleate boiling occurs when steam

bubbles start forming on the surface of the heated fuel rods. These bubbles then detach and rise, causing the coolant to boil. This regime is characterized by the presence of dispersed steam bubbles in the liquid coolant.

Representation of these flow regimes is important for accurate reactor physics applications. Module THM: in Donjon5 provides a simulation of flow regimes in a single assembly of the core. Output of THM: are local parameter values used to interpolate the multiparameter database produced by Dragon5. Modification of THM: is required and should be adequately validated at the Donjon5 level. This validation will involve contributions from and exchanges with the OpenFOAM community, as BWR thermalhydraulics models are of increasing interest across the world. Such models are already integrated with SERPENT2 and may serve as background for this subproject. (Peltola, 2015)

B.3 Investigation of a SMR based on the Molted Salt Reactor concept (M.Sc.A. 3)

We will investigate the Stable Salt reactor concept from Moltex Clean Energy. The molten salt reactor (MSR) is a fast reactor that uses recycled nuclear waste as fuel. This is a class of nuclear fission reactor in which the primary nuclear reactor coolant and the fuel are combined into a molten salt mixture. Unlike traditional nuclear reactors that use solid fuel, MSRs employ a liquid fuel consisting of a mixture of molten salts, typically fluoride or chloride salt. The liquid fuel offers advantages such as better heat transfer and the ability to continuously remove fission products. MSRs have the potential to operate with a closed fuel cycle, where fuel can be continuously processed, removing fission products and adding fissile material. This can improve fuel utilization and reduce the amount of long-lived nuclear waste generated. This reactor concept is the most innovative SMR design considered in Canada. Developing computational schemes for the MSR concept and optimizing fuel supply over centuries of operation is one of the major outcomes of this research proposal.

This M. Sc. A. subproject will focus on reactor physics models including the effect of fuel decay inside and outside the core. We will try to obtain some inputs on fuel from the SMR vendors, such as Moltex, so as to make this study as useful as possible in a Canadian context. A MSR is a very futuristic concept, and many unresolved issues exist now. The long-term fuel supply and reprocessing made possible by MSRs will be investigated in more details by subproject B.5.

B.4 Development of SMR geometry models with the Open CASCADE Technology (OCCT) toolkit (M.Sc.A. 4)

Small modular reactors feature fuel geometries are more complex than those of legacy CANDU or PWRs. A lattice code such as Dragon5 needs to support *non-native* geometries, a class of geometry models that are constructed using an external tool such as the Open CASCADE Technology (OCCT) toolkit. OCCT consists of C++ classes grouped into Packages. They are organized into Toolkits (libraries), and the latest are grouped into seven Modules. You can download Open CASCADE library totally free and use it at any PC with Windows, Linux or OSX.

A few years ago, we developed a Python application based on the OCCT Application Programming Interface (API) to generate PWRs geometries. This 6000-line application takes an XML assembly engineering representation at input and generates a 2D surfacic representation of the PWR assembly at output. This exercise is more a proof-of-concept as PWR assemblies are easily represented using *native geometries* of Dragon5.

The M. Sc. A. project consists of extending the existing Python application to generate boiling water and hexagonal fuel assemblies with specific fuel patterns. This new Python application will support external boundaries, moderator zones, poison cross, water blades, stiffeners and boxes. An example of a non-native geometry currently used with Dragon5 is depicted in Fig. 4. The resulting surfacic representation will be tracked by module SALT: of Dragon5, leading to accurate solutions of the BTE over SMR fuel geometries.

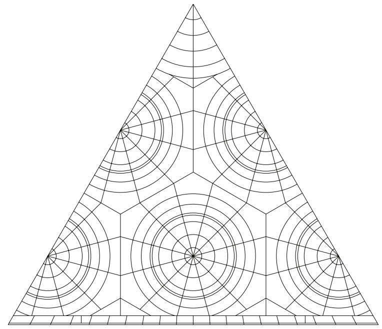

Fig. 4 Example of a non-native geometry in Dragon5

B.5 Simulation of SMR–specific supply chains using CLASS (Ph.D. 1)

CLASS is a dynamic fuel cycle simulation code that uses Dragon5 and Donjon5 reactor simulations with neural networks to analyse complex nuclear power plant operations from fuel fabrication to long-term storage or recycling of spent fuel elements. CLASS is an open-source package of C++ libraries that performs simulations of entire fuel cycles based on several facilities: reactors, cooling pools, fabrication plants, storage and separation plants. It contains a fuel loading model that is used to fabricate fresh fuel from fissile materials. Reactors are simulated through two independent steps: fuel loading followed by irradiation. In conventional CLASS PWR calculations, reactors are simulated by MLP (Multi-Layer Perceptrons) predictors trained on databases generated by Dragon5 (or any other cell code) for fresh fuel discharged after its irradiation cycle is completed. For these neural networks-based approaches, no environment is taken into account. In the last five years, we have coupled CLASS and Donjon5 to perform nuclear scenario simulations involving Uranium Oxyde (UOX) and Mixed Oxyde (MOX) PWR core at equilibrium cycle conditions and we are in the process of modeling PWR based SMR. We now propose to extend this method to a combination of CANDU and SMR reactors.

The methodology at the core of this Ph.D. project is based on the following steps:

1. Collect and understand theDragon5 and Donjon5 reference models for the CANDU and the four SMR designs design investigated by the CNSC-sponsored Alliance grant and by this research proposal. Integrate these contributions in a unified V5-PyKit framework.
2. Generate with Dragon5 the databases required for Donjon5 and CLASS executions.
3. Use CLASS to predict CANDU and SMR spent fuel compositions for definitive storage or after the fuel separation plant using standard PWR fuel reprocessing options.
4. Validate and correct the CLASS models if required.
5. Propose an equilibrium scenario for using reprocessed spent fuel from a reactor concept for use in another type of reactor. Evaluate quantity of fission products to vitrify after passing through reprocessing plant as well as the isotopic contents of the final wastes. Evaluate supply chains of nuclear fuel over long periods of time (centuries) with optimization based on production criteria.

B.6 Introduction of high-performance computing (HPC) capabilities in Dragon5 (Ph.D. 2)

Computer hardware is continuously improving and offers the capability of parallel processing. Modern processors feature up to 128 cores with shared memory that can be used in parallel using the OpenMP API. Moreover, many processors can be used in parallel using the message passing interface (MPI) API. Many numerical algorithms must be reprogrammed using this paradigm in mind. Our investigation will focus on the parallelization of the collision probability (CP) method, of the method of characteristics (MOC) and of the resonance self-shielding models used with deterministic solutions of the BTE.

HPC capabilities must be included at the root of the building blocks provided by Dragon5 to the experts in charge of developing SMR-specific computational schemes.

C. Team

- List the applicant, any co-applicants and key staff of the partner organizations.
- Explain how the knowledge, experience and achievements of these individuals provide the expertise needed to accomplish the project objectives. Discuss the role of each individual and how their contributions, including those of staff from the partner organizations, will be integrated into the project.
- Explain how equity, diversity and inclusion have been considered in the academic team composition.
- For large (average of more than $300,000 per year requested from NSERC) multi-party projects (multiple universities and/or partner organizations), it may be appropriate to provide a description of up to three additional pages detailing university support, governance structure and project management. If applicable, please detail the project manager's qualifications, involvement, role and responsibilities.

The research team includes the applicant and co-applicant (Alain Hébert and Guy Marleau), two external collaborators from University Grenoble-Alpes (Xavier Doligez and Adrien Bidaud), four M.Sc.A students and two Ph.D. students. Alain Hebert and Guy Marleau are the two main developers of the Dragon5 and Donjon5 codes, considered as reference tools in the field of Nuclear Reactor Physics. Knowledge, experience, and achievements of the (co)applicants and of the external collaborators are described below.

Equity, diversity and inclusion (EDI) principles are underlying the recruitment process of HQP at Polytechnique Montréal. Specific training about EDI principles is providing guidance to the academic staff (both academic and administrative) in charge of supporting R&D projects. Specific instances exist at the direction level of Polytechnique Montréal to ensure the strict application of EDI principles.

C.1 Alain Hébert

Alain Hébert is a full professor at Polytechnique Montréal since January 1981. His career is devoted to mechanical statistics of elementary particles and nuclear reactor physics. His actual field of investigation is twofold: (1) Development of innovative computational techniques in nuclear reactor physics and, (2) the application of statistical mechanics to radiation treatment planning (RTP). Alain Hebert R&D in the field of nuclear reactor physics focuses on lattice calculations, including resonance self-shielding models, and on full core simulation tools. Recently, he proposed an application of the legacy approach of nuclear reactor physics to medical applications such as radiation oncology and medical imaging. Alain Hébert will be the main director of every student involved in the Alliance project, with Prof. Guy Marleau as co-director. The Applied Reactor Physics textbook is a major contribution of Alain Hébert (Hébert, 2020). It provides support to graduate-level students at the Institut de génie nucléaire (IGN), introducing state-of-the-art approaches. Applied Reactor Physics is currently the only available textbook at graduate level that supports modern computational schemes used in industry. Starting in September 2010, the Massachusetts Institute of Technology is using it as main textbook for graduate students in Nuclear Science and Engineering. Alain Hébert will act as the academic director of all graduate students and provide close supervision of the M. Sc. A. sub-project B.2 (BWR thermalhydraulics), B.4 (OCCT geometric models), B.5 (Open Cascade support) and on Ph. D. sub-project B.6 related to the HPC implementation.

C.2 Guy Marleau

Guy Marleau is an expert on transport theory and reactor physics. He has been involved in the development and qualification of the code DRAGON since 1986. He has used codes such as Dragon, Donjon, SERPENT and MCNP to model all types of power and small reactors including Canada Deuterium Uranium (CANDU), Pressurized Water Reactors (PWR), High Temperature Reactors (HTR), and two small reactors: ZED-2 and the SLOWPOKE-2. Moreover, along the years he has been involved in more remote projects such as 1) simulating and characterizing neutron detectors, 2) using charge transfer devices for muon detection (both in collaboration with CNL), and 3) characterizing the source term from CANDU reactors for a mobile nuclear laboratory of Health Canada. Starting in 2017, he has established a collaboration with the CLASS code developers from the IN2P3-CNRS research centre in Orsay, France leading to the coupling CLASS to Dragon5 and Donjon5 for scenario analysis of PWR reactor fleet. This team is now in the process of adding to this fleet small PWRs. Guy Marleau will act as co-director on many subprojects, including the supervision of the M. Sc. A. sub-project B.1 and B.3 related to SMR concepts and on Ph. D. sub-project B.5 related to the CLASS scenario simulation package.

C.3 External Collaborators

The two external collaborators are the authors of the CLASS scenario simulator and will play a software integration role. They are members of the University Grenoble-Alpes (IN2P3-CNRS research centre). Among these, Xavier Doligez, a developer of the code CLASS has been involved in scenario studies for over 10 years, both for PWR studies and on recycling irradiated fuels in CANDUs. A second collaborator to the team is Adrien Bidaud, also a contributor to CLASS, that has recently been working on generalized perturbation theory in Monte Carlo neutron simulations for applications to resonance parameters studies, PWR scenarios with multiple recycling studies in CLASS as well as waste minimization in sodium-cooled fast reactors and thorium nuclear data for molten salt reactors.

Training plan

- Indicate how the knowledge and experience gained by research trainees and the partners' staff members are relevant to the advancement of the field, to applying knowledge or to strengthening the partners' sectors.
- Describe how the project and the partnership offer opportunities for enriched training experiences that will allow research trainees (undergraduates, graduates and postdoctoral fellows) to develop relevant technical skills as well as professional skills, such as leadership, communication, collaboration and entrepreneurship. Include the nature of the planned interactions with the partners and other relevant activities.
- Explain how equity, diversity and inclusion are considered in the training plan (see here for guidance).

The knowledge and experience gained by the graduate students involved in this Alliance project will contribute to increasing R&D capacity in the field. It is our policy to pursue our research activities in close relationship with stakeholders. We provide specific training related to develop (under strict *quality assurance* guidelines), support, use and promote production software related to nuclear reactor physics. We are the only university in Canada with such a capability. Stakeholders from Canada and from elsewhere in the world are searching for trainees with similar skills. As of writing, we cannot fulfill all industry needs.

Dragon5 and Donjon5 are unique codes in the world. Dragon5 is the unique Open-Source lattice code and the only developed in a University context. They are the only actual option available in Canada for supporting future needs in reactor physics. Other Canadian universities use these codes, but Polytechnique Montréal is the only university in charge of continuous integration of new developments.

This Alliance proposal will contribute to the training of highly qualified personnel (HQP). Four additional M.Sc.A. and two additional Ph.D.s nuclear engineers will be trained and become available to the nuclear industry in Canada. Some of our graduate students are performing 6-to-8-month internships in stakeholder organizations, working on their dissertation or thesis subject in an industrial environment. In this case, the internship is covered by an Internship Agreement between Polytechnique Montréal and the organization. Advances made with the help of this Alliance proposal are therefore subject of interest for the industry and training gained by the students are well suited to fit industrial needs. During the past six years, I personally trained more than 7 M.Ing. students, 16 M.Sc.A. students and 8 Ph.D. students.

Improving simulation tools is important for developing and implementing innovative SMR concepts. We are developing tools and capabilities to perform deterministic computations in support to safety assessment: criticality studies, core simulation in normal operation and production of macroscopic cross-section libraries for multi-physics tools that are used by accident simulations. Scenario simulations based on neural networks will permit an optimal deployment of full-scale and SMR plants to manage uranium resources, reduce wastes and proliferation.

In our groups, and in this collaboration, respect and communication are priorities and everyone involved has the right to express their opinions and live according to their cultures. Based on our institutional principles, we have established the 4 priorities in our collaboration with regards to EDI: 1) Recognize the importance of diversity within the collaboration. Our team combines various expertise: physics, engineering, and medicine. We insist that each professor be an example of inclusion for students in training to follow. 2) Correct inequalities. In order to give an equitable opportunity to all students, whatever their identity, we need to enhance diversity in the composition of the HQP involved in the project, through open hiring policies and inclusive practices. Many of our graduated students in the past are from underrepresented groups. 3) Respect the identity of each individual. Each member of our collaboration is invited to live openly and to respect others. Each student has an equal status in out Live Lab organization. 4) Provide free support for Dragon5 and Donjon5 users in underdeveloped countries, as we are developing one of the only deterministic options for them. We offer a fast-track to integrate students from these countries in our teams.

Underrepresented groups face a variety of well-documented challenges, including stereotypes, unconscious biases, limited role models and mentoring, unfair recruiting, as well as bias in grants, awards, and speaker invitations. The IGN already features a diverse class of students (including females and visible minorities). Following the training I took in 2019 at Polytechnique Montréal and online on EDI, I made changes to my recruitment methods for members of the *Institut de Génie Nucléaire* (IGN). Seamless integration is difficult for international students who face challenges like cold weather and difficulties with the English or French languages. We offer a welcome kit that contains various information such as the French and English courses offered at Polytechnique Montréal. We pair new international students with another international student in the IGN before arriving at our city to discuss integration strategies. We allow flexible working hours and accommodation for remote participation (via Zoom) to our Live Lab. Team members follow published best practices for hiring and retention. Trainees are recruited at different levels and programs for greater diversity. Presentations to various groups ensure visibility for these models and links to potential recruits. In particular, physics and engineering experience an under-representation of women at all university levels. We take actions to help change this portrait: (1) We target organizations like Poly-FI for the recruitment of female students (2) We do canvassing to specific institutions such as the *École Polytechnique Féminine* (EPF) in France.

D. References

- Use this section to provide a list of the most relevant literature references. Do not refer readers to websites for additional information on your proposal. Do not introduce hyperlinks in your list of references.
- These pages are not included in the page count

Hébert A. and Roy R. The Ganlib5 kernel guide (64–bit clean version), IGE-332 [Report]. - [s.l.] : Polytechnique Montréal, 2022.

Hébert A. Applied Reactor Physics [Book]. - [s.l.] : Presses Internationales Polytechnique, 2020.

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MacFarlane R. E. and Kahler A. C. Methods for Processing ENDF/B-VII with NJOY [Journal] // Nuclear Data Sheets, 111. - 2010. - p. 2739.

Marleau G., Hébert A. and Roy R. A user guide for Dragon version5, IGE-335 [Report]. - [s.l.] : Polytechnique Montréal, 2023.

Mouginot B. [et al.] Core library for advanced scenario simu- lation, CLASS : principle & application [Conference] // The Role of Reactor Physics toward a Sustainable Future"(PHYSOR 2014). - 2014. - p. 12.

Okuno H., Naito Y. and Suyama K. OECD/NEA Burnup Credit Criticality Benchmarks Phase IIIB: Burnup Calculations of BWR Fuel Assemblies for Storage and Transport," JAERI-Research, Report 2002-001 NEA/NSC/DOC(2002)2, February [Report] / OECD/NEA. - 2002. - Report 2002-001 NEA/NSC/DOC(2002)2.

Peltola Juho CFD Modeling of Heat Transfer, Boiling and Condensation: NUFOAM & NUMPOO [Conference]. - Espoo : SAFIR2014 Final Seminar, 2015.

Personal identification no. (PIN)	Family name of applicant
Valid 13665	Hébert

PROPOSED EXPENDITURES					
	Cash				
	Year 1	**Year 2**	**Year 3**	**Year 4**	**Year 5**
1) Salaries and benefits					
a) Students	91,000	93,000	95,000	97,000	0
b) Postdoctoral fellows	0	0	0	0	0
c) Technical/professional assistants	0	0	0	0	0
d)	0	0	0	0	0
2) Equipment or facility					
a) Purchase or rental	0	0	0	0	0
b) Operation and maintenance costs	0	0	0	0	0
c) User fees	0	0	0	0	0
d) *Computrer support*	2,000	2,000	2,000	2,000	0
3) Materials and supplies					
a)	0	0	0	0	0
b)	0	0	0	0	0
c)	0	0	0	0	0
4) Travel					
a) Conferences	6,000	4,000	2,000	0	0
b) Field work	0	0	0	0	0
c) Project-related travel	0	0	0	0	0
d)	0	0	0	0	0
5) Dissemination					
a) Publication costs	1,000	1,000	1,000	1,000	0
b)	0	0	0	0	0
6) Technology transfer activities					
a)	0	0	0	0	0
b)	0	0	0	0	0
c)	0	0	0	0	0
Total Proposed Expenditures	100,000	100,000	100,000	100,000	0
Partner organization recognized for cost-sharing	50,000	50,000	50,000	50,000	0
Partner organization not recognized for cost-sharing					
Other funder (not involved in the research)					
Postsecondary institution					
Amount requested from NSERC	50,000	50,000	50,000	50,000	0

PROTECTED B WHEN COMPLETED

E. BUDGET JUSTIFICATION

E.1 Salaries

Note that any reduction on this budget item will result in reduction in sub-projects that will be realized and reduction in development and publications capabilities. A Gantt diagram is presented as Fig. 1.

M.Sc.A. students

4 M.Sc.A. students (one for each of the first four sub-projects) will be supported by this grant. The first 2 M.Sc.A. students will be hired at the availability of funding and the third and fourth M.Sc.A. students will be hired two years later. M.Sc.A. programs, including lectures and research project, are expected to be completed in 2 years.

Ph.D. students

2 Ph.D. students (one for each of the last two sub-projects) will be supported by this grant.

sub-project		year			
		1	2	3	4
B.1	M.Sc.A. student 1	$21,000	$21,500	–	–
B.2	M.Sc.A. student 2	$21,000	$21,500	–	–
B.3	M.Sc.A. student 3	–	–	$22,000	$22,500
B.4	M.Sc.A. student 4	–	–	$22,000	$22,500
B.5	Ph.D. student 1	$24,500	$25,000	$25,500	$26,000
B.6	Ph.D. student 2	$24,500	$25,000	$25,500	$26,000
total		$91,000	$93,000	$95,000	$97,000

1: Investigation of a SMR based on the Boiling Water Reactor concept − neutronics
2: Investigation of a SMR based on the Boiling Water Reactor concept − thermal hydraulics
3: Investigation of a SMR based on the Molted Salt Reactor concept
4: Development of SMR geometry models with the Open CASCADE Technology
5: Simulation of SMRspecific supply chains using CLASS
6: Introduction of high-performance computing (HPC) capabilities in Dragon5

E.2 Computer equipments and expenses

A budget of $2,000 per year will be spent for computer hardware, computer support from the *computer services* of Polytechnique Montréal, software licenses and furniture.

E.3 Conferences

A averaged budget of $3,000 per year will be spent to cover the costs of participations to Canadian (CNS–sponsored) and international conferences (Physor and M&C meetings). We encourage participation of graduate students.

	year			
	1	2	3	4
meetings	$6,000	$4,000	$2,000	–

E.4 Publications

A budget of $1,000 per year will be spent for covering the costs of publication in *Nucl. Sci. Eng.* and *Ann. Nucl. Energy*.

Personal identification no. (PIN)	Family name of applicant
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Organization Category

Partner organization recognized for cost-sharing

Partner organization

Natural Resources Canada

Partner department

Nuclear Energy

Contact family name, contact given name

Poupore, Jessica

Contact email address

jessica.poupore@nrcan-rncan.gc.ca

CONTRIBUTIONS FROM PARTNER ORGANIZATION

	Year 1	Year 2	Year 3	Year 4	Year 5
Cash contributions to direct costs of research	50,000	50,000	50,000	50,000	0
In-kind contributions					
1) Salaries for scientific and technical staff	10,000	10,000	10,000	10,000	0
2) Donation of equipment, software	0	0	0	0	0
3) Donation of material	0	0	0	0	0
4) Field work logistics	0	0	0	0	0
5) Provision of services	0	0	0	0	0
6) Use of organization's facilities	0	0	0	0	0
7) Salaries of managerial and administrative staff	0	0	0	0	0
8)	0	0	0	0	0
Total In-kind contributions	10,000	10,000	10,000	10,000	0
Contribution to postsecondary institution overhead	0	0	0	0	0

Contributions from Partner:

NRCan (Nuclear Energy Division) will provide in kind support in administering and managing the proposed work, taking part in research design and interpretation of the data and in the work to review reports and disseminate the information. This is estimated at around 50 hours per year. NRCan will also make an "in kind" contribution in salary (for the time allocated to the discussions in virtual meetings) and travel costs for staff to the annual UNENE Workshop. The members from NRCan-NED that are involved in this project are Jessica Poupore (Senior Advisor), Sara Arab (S&T Analyst), Jenny Cox (Senior Advisor), and Daniel Brady (Deputy Director).

It is expected that Nuclear Energy Division staff will meet with the principal investigators on an annual basis to discuss the progress/results and research plans, and also take into account implications for policy and decision making to ensure the data is relevant for end-users. A wrap-up meeting at the end of the project is also expected to take place.

The principal investigators and the HQPs of the project will also meet NED staff at UNENE and other conferences to discuss the implication of the results. There is also potential for a workshop convening all projects under the NSERC-NRCan partnership, likely to take place on the margins of an existing event.

NRCan is the implementing agent of the Generation IV International Forum (GIF) framework in Canada and nominates and coordinates the participation of Canadian organizations in various multilateral collaborative research activities related to development of advanced nuclear reactors. As an additional service contribution, NRCan can provide information about the GIF publications relevant to the proposed project.

Table 1: Financial contribution from Natural Resources Canada

Partner Organization	Cash/$/year	In kind/$/year
NRCan – Nuclear Energy Division	50,000	10,000

Reviewer Suggestions
(Form 101)

Date
2023/08/10

Family name of applicant	Given name	Initial(s) of all given names	Personal identification no. (PIN)
Hébert	Alain	A	**Valid** 13665

Title of proposal
Small modular reactors: Characterization of fuel and multi-year simulation of operation

#	Reviewer	Area(s) of expertise	PIN	Lang.
1	Pioro (Igor) Faculty of Engineering and Applied Science Ontario Tech 2000 Simcoe Street North Osawa, ON CANADA L1G0C5 1 (905) 7218668 ext 5528 igor.pioro@ontariotechu.ca	Heat engineering, Nuclear engineering, Nuclear fuel/power, Renewable energy, Thermal sciences		
2	Nichita (Eleodor) Faculty of Engineering and Applied Science Ontario Tech 2000 Simcoe Street North Osawa, ON CANADA L1G0C5 1 (905) 7218668 ext 5527 eleodor.nichita@ontariotechu.ca	Mathematical modelling, Neutron/radiation transport, Neutronic design, Nuclear reactor kinetics/control,		
3	Dumonteil (Éric) Département de Physique Nucléaire Commissariat à l'Énergie Atomique et aux Énergies A Institut de Physique Théorique Orme des Merisiers bâtiment 774 Gif-sur-Yvette Cedex FRANCE 91191 11 (33) 169086000 eric.dumonteil@cea.fr	Nuclear reactors, statistical mechanics, uncertainty quantification, Monte Carlo, code Geant4, Perturbations theory		
4	Arsenault (Benoit) NS&L Kinectrics Inc. 393 University Ave. Toronto, ON CANADA M8Z5G5 1 (416) 8739051 benoit.arsenault@kinectrics.com	Reactor physics, Safety assessment, Reactor design, Lattice calculation		
5	Sissaoui, M. (Tahar) Reactor Core Physics Department Candu Energy Inc. (SNC-Lavalin) 2251 Speakman Drive Mississauga, ON CANADA L5K1B2 1 (905) 8239040 ext 36457 Tahar.Sissaoui@snclavalin.ca	Reactor physics, Safety assessment, Reactor design, Lattice calculation		

Personal identification no. (PIN)	Family name of applicant
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PARTNER ORGANIZATION CONTACT INFORMATION

Family name, given name, Initial(s)	Position or title	Telephone
Poupore, Jessica, R	Senior S&T advisor	(613) 2928981 ext
Email address jessica.poupore@nrcan-rncan.gc.ca		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		
Family name, given name, Initial(s)	**Position or title**	**Telephone**
Email address		

Xavier Doligez is a researcher from the Laboratory of Subatomic Physics and Cosmology (LPSC), a unit of the Centre national de la recherche scientifique (CNRS) in collaboration with the Université Grenoble-Alpes (UGA). He is collaboration with the Université Paris-Saclay and with the Université Grenoble-Alpes (UGA). He is a developer of the code CLASS has been involved in scenario studies for over 10 years, both for PWR studies and on recycling irradiated fuels in CANDUs. His research focuses on many subjects related to the nuclear reactor physics for legacy or advanced reactors.

Adrien Bidaud is a professor at the Université Grenoble-Alpes (UGA). He is also a contributor to CLASS that has recently been working on generalized perturbation theory in Monte Carlo neutron simulations for applications to resonance parameters studies, PWR scenarios with multiple recycling studies in CLASS as well as waste minimization in sodium-cooled fast reactors and thorium nuclear data for molten salt reactors. His research focuses on Nuclear Reactors, Nuclear Fuel, Energy Economics, Thorium, Actinides, Plutonium, Uranium, Depleted Uranium, Accelerator Driven Systems (ADS), Nuclear Science, Experimental Nuclear Physics, Nuclear Fission, Nuclear Engineering and Nuclear Energy.