National Research Foundation

PRIME MINISTER'S OFFICE SINGAPORE

ARTIFICIAL INTELLIGENCE (AI)-FOR-SCIENCE (AI4S)

Catalytic Grant Call Information Sheet

Call-for-Proposals

1 Objectives

- 1.1 The National Research Foundation (NRF) Al-for-Science (Al4S) Funding Scheme seeks to support collaborative teams of scientific domain and Al researchers, to pursue cutting-edge basic science in Singapore which will significantly advance the development of Al methods and tools for scientific research, and leverage these Al solutions to make a transformative stepchange in scientific discovery¹.
- 1.2 The AI4S Catalytic grant scheme will provide funding support of up to \$2 million for 2 to 3-year projects. It will invite proposals to pursue cutting-edge basic science, that will advance knowledge in scientific discipline(s) and AI methods and tools for scientific research. Proposals at the intersection of multiple scientific disciplines are encouraged, including but not limited to: physics, chemistry, biology, materials science, earth/climate science, complexity science, computer science, and mathematics².
- 1.3 The AI4S Catalytic scheme aims to stimulate new collaborations between AI and scientific domain researchers, to allow Singapore to be responsive to rapid advancements in AI for Science, and to support a large base of activity in AI for Science which could feed into future programmatic grant calls. Proposals in novel, emerging research areas at the convergence of AI and scientific discovery, including scientific domains where the application of AI is still nascent but could enable transformative progress, are encouraged.
- 1.4 Beyond research outcomes, the AI4S scheme is intended as a platform to convene global talent and cultivate a new generation of interdisciplinary experts who are proficient in both AI technologies and scientific domains. It is intended to foster a community of AI-literate scientists who can apply advanced computational methods to address complex research challenges and bridge the gap between AI and various disciplines for accelerated scientific discovery and problem-solving.

¹ A transformative step-change in scientific discovery includes but is not limited to: i) accelerating the time taken for scientific discovery (e.g. by two-orders of magnitude (100x) or greater); or ii) enabling significantly larger or more complex hypothesis spaces to be explored; or iii) enabling scientific discoveries which would otherwise be prohibitively difficult or impossible (with reference to a traditional baseline process).

² The AI4S Catalytic grant scheme is not intended for (i) epidemiological and behavioural studies; (ii) observational studies (including cohort, longitudinal, case-control studies, etc.); (iii) clinical and drug trials; (iv) health services research/operations research; (v) infrastructure/facilities set-up; and (vi) market/drugs/product development.

2 Eligibility

Host Institutions

- 2.1 Institutions/organisations which fulfil the following criteria will be eligible as a host institution³:
 - Registered as a Singapore Autonomous University, A*STAR Research Institute, or CREATE Entity;
 - Has adequate research infrastructure to support research activities; and
 - Has an Office of Research, Director of Research and Finance department to fulfil the responsibilities of a research grant recipient.

Team Composition

- 2.2 Research teams are expected to be multi-disciplinary, and should include:
 - Two Co-Lead PIs, possessing relevant expertise in one or more scientific domain(s) and AI respectively.
 - Team PIs and collaborators possessing relevant expertise in one or more scientific domain(s) and AI.
- 2.3 Co-Lead PIs and Team PI(s) must fulfil the following requirements at the point of application and throughout the project duration:
 - Hold a primary and/or joint appointment(s) at eligible host institution(s)/organisations(s), polytechnic(s) or public healthcare institution(s), with a minimum time commitment of 9 months (per calendar year) in Singapore; and
 - Be an accomplished PI with a track record of leadership ability in coordinating research program(s) and providing mentorship to research teams(s), as well as having productive research outcomes.
 - As a guideline, Co-Lead PIs should commit 10-20% of their time, and Team PIs should commit 10% of their time to the project, respectively.
- 2.4 International PI(s) who do not fulfil the above requirement may participate as Co-Lead/Team PI(s), but are expected to have reasonable time commitment for conducting research activities within Singapore, and contributing to the aims of the project. As a guideline, International Co-Lead PIs should commit 10-20% of their time, and International Team PIs should commit 10% of their time to the project, respectively. This time commitment can be fulfilled by conducting research activity in Singapore, and remotely.
 - Residency of international PI(s) in Singapore may be budgeted for in the proposal and is supportable by the grant. Eligible items for residency include travel, accommodation, and cost of living allowance (to cover meals,

³ One host institution is to be identified per proposal/project team. The Host Institution is the primary institution addressed in the Letter of Award which will receive the grant funding, and be responsible for the management of awarded projects, including the collation of expenses and disbursement of funds on behalf of participating institutions of Team PI(s).

transport, incidentals). <u>Please note that the salary of international PI(s) will not be supportable under the AI4S Catalytic Grant</u>.

- 2.5 Private sector and other entities can participate as collaborators.
 - International PI(s) participating in the project as Collaborators may be Visiting Experts, that can be budgeted for in the proposal and are supportable by the grant. Eligible items for Visiting Experts include travel, accommodation and honorarium.

3 Selection Process and Evaluation Criteria

- 3.1 Proposals will be selected through a two-stage process based on scientific excellence and merit:
 - <u>Stage 1 Video & Slides Evaluation:</u> Evaluation at this stage would be done
 by the AI4S Evaluation Panel (EP) based on a concise summary of the
 proposed research idea, as presented in a video and accompanied by
 presentation slides. The EP would be able to refer to the Full Proposal
 document, and could be assisted (if necessary) by International Peer
 Reviewers. Shortlisted proposals will immediately proceed to Stage 2
 evaluation.
 - Stage 2 Full Proposal Evaluation: Evaluation of the Full Proposal would be done at this stage by the AI4S Evaluation Panel (EP) and International Peer Reviewers. Selected applicants will be invited for an interview at a virtual meeting with the AI4S EP, and proposals will be selected for award based on the evaluation outcomes.
- 3.2 Applicants are required to submit <u>both</u> the Stage 1 (Video & Slides) and Stage 2 (Full Proposal) materials together, during the grant call's submission window, to facilitate a shorter review cycle.
- 3.3 The proposals will be evaluated based on:
 - <u>Video & Slides</u>: (i) originality and ground-breaking nature of the research;
 ii) significance and potential impact of the research;
 iii) scientific approach.
 - <u>Full Proposal</u>: (i) originality and ground-breaking nature of the research; (ii) significance and potential impact of the research; (iii) scientific approach; (iv) technical competencies of the team.
- 3.4 Co-Lead PIs and Team PIs are expected to commit a proportionate amount of their time in ensuring the success of the project. The time commitment of each team member dedicated to the project will be assessed as part of the evaluation criteria.

4 Co-location of Research Teams

4.1 Space will be provided at the National Research Foundation Campus for Research Excellence and Technological Enterprise Campus (CREATE) for projects funded through AI4S. Co-location of teams is intended to: (i) foster strong interactions between AI and Domain scientists; (ii) facilitate hosting of overseas partners; (iii) facilitate sharing of resources and supporting platforms with active programme management to maximise research synergies and impact of research outcomes. As a default, researcher staff supported through AI4S will be primarily based in the co-located space, except where there is a need for proximity to existing resources.

5 Indirect costs

5.1 Fixed percentage of 15% indirect costs will be awarded to Host Institutions (HIs), in view that services and utilities charges will be waived for awarded projects, which will be co-located in facilities within NRF CREATE.

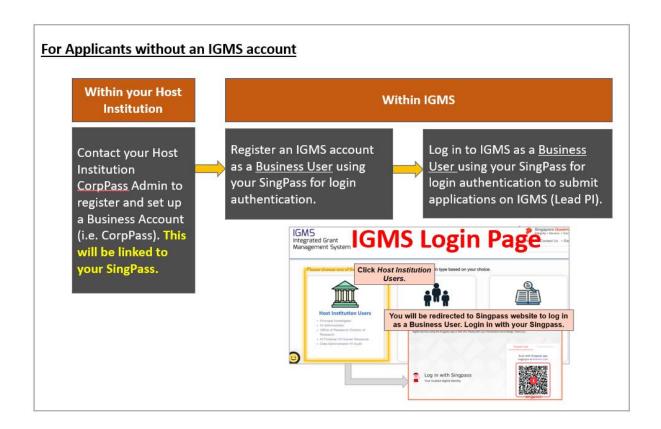
6 Intellectual Property Rights

6.1 The HI will oversee management of Intellectual Property (IP), and IP and commercialisation approach for each project is to be jointly agreed upon between the host and partner institutions. The HIs are to reserve a royalty-free, irrevocable, worldwide, perpetual, and non-exclusive right for the Singapore Government (and affiliated public sector agencies) to use the Research IP for their statutory functions, non-commercial and/or R&D purposes.

7 Submission of Application

- 7.1 All interested applicants must apply via the Integrated Grant Management System (IGMS) (URL: https://www.researchgrant.gov.sg). The system will be opened to accept submissions from 20 August 2025 (Wednesday). 0900hrs SGT.
- 7.2 All applications must be submitted by the Co-Lead PI and endorsed by the Host Institution's Director of Research (DOR) via the IGMS by 14 October (Tuesday), 1600 hrs SGT. Applicants are encouraged to submit the complete application early, in order to allow the DOR to endorse the proposal on IGMS in a timely manner. Please refer to Appendix A on pointers for writing the AI4S Catalytic proposal.
- 7.3 Prior to the submission, Co-Lead Pls and Team Pls are required to have a registered IGMS account as a Business User with an eligible Host Institution. This is required for the Co-Lead Pl from the Host Institution to submit the application on behalf of the project team, and the remaining Co-Lead Pl/ Team Pls to be added as team members in the application on

IGMS. For new applicants **without** an IGMS account, please refer to the flowchart below for the steps to register for an IGMS account and log in to IGMS.



- 7.4 Please note that the online IGMS application form will require each applicant to have an authorised ORCID ID on their IGMS User Profile Page to create an application as a Co-Lead PI or be listed in an application as a Team PI.
- 7.5 Applicants must complete the online IGMS application form and upload the Video + Slides, Full Proposal Application Forms (please use the template in **Attachments 1 to 3**) and Annex under the *Research Proposal* section of the IGMS application.

8 Details of Research Proposal Documents

8.1 This section provides the details of the main documents related to the proposal submission. Please refer to Paragraph 9.5 for the complete list of submission requirements.

8.2 Video:

- (a) A video recording of your presentation, presenting a concise summary of your Research Proposal.
- (b) The video should cover the following content: Research Objectives, Competitive Scan, Approach, and Outcomes and Deliverables. Please see **Attachment 1** (Application Form for Stage 1).

- (c) The video must not exceed **12 minutes**, or your application may be rejected without review.
- (d) The video file format should not exceed 500MB and should be compatible with Windows Media Player (e.g. MP4 video file, QuickTime movie file, etc). Microsoft PowerPoint format can also be used.
- (e) The video must be uploaded to a cloud storage with a generatable link, made accessible and downloadable by external parties, and have at least 6-months validity. The link must be provided in Attachment 1. Broken or inaccessible links may lead to application being rejected without review.

8.3 Slides:

- (a) A copy of the presentation slides used in the Video (guiding template in **Attachment 2**).
- (b) The slides must be converted to <u>PDF format</u> and uploaded in the *Research Proposal* Section of IGMS.
- (c) The slides cannot exceed **10 pages** (excluding the Cover slide). Use <u>at least</u> Arial Font Size 12 for all text and figures, and standard slide sizes. [Note: There is no cap on the number of slides in the Video presentation. If the total slide number in the Video exceeds 10, the copy of the presentation slides must be shortened/summarized to meet the 10-slides limit with no additional information]. Please ensure the final PDF file does not exceed 4 MB.
- (d) All supplementary information, limited to figures, tables, charts or diagrams ONLY, and referenced in the Video and Slides, must be appended to the **Annex** (see <u>Paragraph 8.5</u>) that is uploaded to IGMS as a separate document.
- (e) Please note that the content in the Slides is only meant to facilitate the EP's review of the Video.

8.4 Full Proposal:

- (a) The Full Proposal should address the adapted Heilmeier's questions (**Appendix A**). Please use **Attachment 1** (Full Proposal Template) to develop the Full Proposal.
- (b) The contents of the Full Proposal must not exceed **15 pages** (excluding cover sheet and annexes) and be written in Arial font size 12 with single line, normal spacing and normal margins. All figures, charts and tables should be consistently labelled.

8.5 Annex:

- (a) References and a Gantt Chart are mandatory and must be included in the Annex. The Gantt Chart should contain details of the key research activities, go/no-go decision points, measurable key deliverables, and their timelines.
- (b) All supplementary information, limited to figures, tables, charts or diagrams ONLY, must be referenced in the Video, Slides or Full Proposal and appended to the Annex.

9 Steps to follow in the Integrated Grant Management System (IGMS)

- 9.1 Please complete the application by navigating to *Grants > Open Grant Calls > AI4S Catalytic Grant Call > Apply*.
- 9.2 All sections in the IGMS application form should be filled up completely as it will serve as the official summary of the proposal being submitted for consideration.
- 9.3 Please refer to the **IGMS Training Guide for Potential Applicants** (under "Help" section in IGMS home page) for guidance on the application process.

Section 1 - Research Details

- 9.4 This section of the IGMS application form includes the following:
 - a. Project duration (months) (note: maximum duration: 36 months);
 - b. Title of Research Project (note: maximum 2000 characters);
 - c. Institution;
 - d. Keywords of proposal (note: up to 6 keywords, separated by semicolon ":"):
 - e. Main research area;
 - f. Potential application/exploitation of research (Note: please be concise and keep to 100 words);
 - g. HRCS Coding (note: only applicable to proposals which are in the Health and Biomedical Sciences research area);
 - h. Scientific Abstract (Note: please be concise and keep to 300 words);
 - i. Lay Abstract (Note: please be concise and keep to 300 words); and
 - j. Research Proposal (Note: The Video, Presentation Slides, Full Proposal and Annex should be uploaded at this section. Please refer to Paragraph 9.5 for details.)

Research Proposal

9.5 The following attachments in <u>PDF format</u> should be uploaded at this section of the IGMS application form <u>using the filenames as listed in blue</u>:

Table 1. Documents for Submission

Document	Remarks for Submission Requirement	Format of Filename	Description
Video	Mandatory	01 Al4S Catalytic Video <input co-<br=""/> Lead Pl Names>	Please use the template and follow the instructions in Attachment 1 . Video cannot exceed 500MB in size. Please read Paragraph 8.2.
			Note: Video Link must be inserted into the application form (Attachment 1).
			Note: Please ensure Co-Lead PI, Team PIs and Collaborators sign on the Declaration Page.

Document	Remarks for Submission Requirement	Format of Filename	Description
Presentation Slides	Mandatory	02 AI4S Catalytic Presentation Slides <input co-lead="" pi<br=""/> Names>	Please use the template and follow the instructions in Attachment 2. Please read Paragraph 8.3.
Full Proposal	Mandatory	03 AI4S Catalytic Full Proposal <input co-lead="" pi<br=""/> Names>	Please use the template and follow the instructions in Attachment 3 . Please read Paragraph 8.4.
Annex	Mandatory for (a) - (f). Optional for (g)	04 Al4S Catalytic Annex to Full Proposal <input co-lead="" names="" pi=""/> (a) References (b) Write-up on Related Grant(s) (c) Gantt Chart (d) Proposed Performance Indicators (e) Talent Development Plan (f) Ethics Statement (g) Figures, Charts, Diagrams or Tables only (optional)	This is one continuous document attached as a single file. Please use clear Headings for Sub-Sections a) to c). Final file size must not exceed 4 MB. (a) References: a listing of all references listed in the Full Proposal application. Please include the full titles and DOI numbers of the publications listed. Do not forget to reference your own key publications related to the proposal (if any). [Note: Hyperlinks not necessary]. (b) Write-up on Related Grant(s) Describe the research funded by currently held grant(s), and how the objective and research differ from that in the AI4S application. Please refer to Attachment 3 for the format of reporting. (c) Gantt Chart Provide a Gantt Chart (appropriately referenced in the Full Proposal) with details on the key research activities and go/no-go and measurable key deliverables and their timelines. (d) Proposed Performance Indicators Provide in a table the following: Number of publications Number of conference proceedings Number of conference proceedings Number of conference proceedings Number of publications in top 10% most highly cited sources by field (e.g. journals or other equivalent publications) worldwide

Document	Remarks for Submission Requirement	Format of Filename	Description
			4. Number of postdoctoral fellows trained5. Number of Masters and PhD students trained
			(e) <u>Talent Development Plan</u>
			Describe plans for cross-training of researchers in AI and domain sciences and long-term adoption of AI within the domain. (Maximum 1 page, excluded from proposal page limit.)
			(f) Ethics Statement
			Provide a statement on the potential ethical impacts and risks of the application of AI in the proposed research. Submissions should also address how these risks can be managed and mitigated. (Maximum 1 page, excluded from proposal page limit.)
			(g) Any other figures, charts, diagrams or tables only.
			They should be clearly labelled and appropriately referenced in the Full Proposal.

Note: Annexes will not count towards the limit of 15 pages for the Full Proposal.

Section 2 – Research Team, Collaborators, Referees

- 9.6 This section is to update the relevant information for all team members (**Co-Lead Pls, Team Pls and Collaborators**) participating in the research. These should be the same team members reflected in the cover sheet of the Research Proposal.
- 9.7 The Co-Lead PIs can search the Team PI(s) by using Name / E-mail / ORCID. (Note: only the role 'Team PI' should be used, and the role 'Co-Investigator' should not be used for the AI4S application).
- 9.8 Please ensure that the "% effort within this project" for all team members (Co-Lead PIs, Team PI(s) and Collaborator(s)) adds up to 100%.
- 9.9 Applicants must provide the CVs of all the team members (Co-Lead Pls, Team Pls and Collaborators) in this section on IGMS, during the Whitepaper and Full Proposal stages. Please use the format in **Appendix B** and name

the files using the filenames in blue below. Note: Please do not add any underscores to the filenames.

05 Al4S Catalytic CV Co-Lead PI < Insert Co-Lead PI Name>
05 Al4S Catalytic CV Team PI < Insert Team PI Name>
05 Al4S Catalytic CV Collaborator < Insert Collaborator Name>

9.10 For Co-Lead PIs and Team PIs, please upload the CVs as individual attachments under *Research Team*, *Collaborators*, *Referees* section of the IGMS application. For collaborators, please upload the CVs under *Other Attachments* section of the IGMS application.

Section 3: Research Milestones

9.11 The team should provide relevant research milestones and their proposed duration in this section. These milestones should be key technical milestones and should be as quantitative as possible as measures of success at midterm and completion.

Section 4: Budget

- 9.12 The total requested budget should reflect a realistic estimation of the project needs and be fully justified. The overall level of the grant offered will be determined on the basis of the needs and judged by the peer reviewers and Evaluation Panel against the requested budget.
- 9.13 The budget categories applicable for Al4S are: (i) Expenditure on manpower (EOM); (ii) Other operating expenses (OOE); (iii) Equipment (EQP); (iv) Overseas travel (OT); and (v) Research scholarship (RS). Note: RS category is not eligible for indirect costs.
- 9.14 The team may also refer to the Budget Checklist (**Appendix C**) and Nonfundable Direct Costs list (**Appendix D**) for a guide on budgeting.
- 9.15 HPC Compute Budget (if applicable): Applicants should include a comprehensive HPC Compute Budget for the entire project cycle in their research proposals, based on current Cloud Service Provider (CSP) rates. The budget should be sufficient to cover the projected HPC resource demands.
- 9.16 Fund disbursement for the Al4S Catalytic grant would be done through a reimbursement basis.

Section 5: Funding Support

9.17 Details of all local grants currently held or being applied for by the Co-Lead Pls and all Team Pl(s) who are expected to receive funding from NRF under the proposed programme, in related areas of work, must be declared in this section.

Section 6: Reviewers

- 9.18 Each Full Proposal submission may include recommendations of international peer reviewers (local reviewers should not be listed), who could potentially be requested to evaluate the Full Proposal. In submitting recommendations for international peer reviewers, the team must ensure that the recommended reviewers:
 - a. Are experts in the subject matter and capable of offering unbiased expert opinions on the scientific merit of the proposed programme;
 - b. Have broad knowledge of the field that will enable them to evaluate the broader multi-disciplinary, educational and societal impact (including economic and other benefits) of the proposed programme;
 - Have good knowledge of global developments in the field to be able to evaluate the international competitiveness of the proposed programme; and
 - d. Have no relationship, direct or otherwise, with any of the team members that would create a real or perceived conflict of interest⁴.
- 9.19 The team may also suggest reviewers who should not be invited to review the proposal.

Section 7: Declaration of Ethics Approval

9.20 The team should declare the requirements of ethics accordingly in this section, if applicable.

Section 8: Other Attachments

9.21 This section may be used to attach supporting documents other than those listed in Section 1: Research Details > Research Proposal.

Section 9: Undertaking

9.22 The Submission should contain all relevant information required for a proper and complete evaluation of their merits without the need to go back to applicants for additional information. Relevant privileged or confidential information should be disclosed if necessary, to help convey a better understanding of the proposed project. However, such information should be clearly marked in the proposal.

⁴ In particular, a reviewer is not permitted to take part in the review of a proposal that originates from his/her home institution (i.e., if the Lead PI or Team PIs of the proposals are from his/her home institution); or if any of the proposal's personnel are closely related to the reviewer, e.g., household family members, partners or professional associates including thesis advisor/advisees; or if the reviewer has a financial interest in the proposing institution, e.g. ownership of stock or securities, employment or arrangements for employment; or if the reviewer or his/her professional associates (e.g., from his/her home institution) have submitted substantially similar proposals for the same grant call.

9.23 Upon completion of the application, the Co-Lead PI should select the acknowledgement button to submit the application to your Host Institution's Office of Research for verification. Please ensure that your application is endorsed by the DOR by **14 October 2025 (Tuesday). 1600 hrs SGT**.

10 Completeness Check

- 10.1 The Co-Lead Pl's Host Institution's Office of Research should perform a completeness check when verifying the submission on IGMS. Please refer to Appendix E for a non-exhaustive guiding checklist for completeness check. NRF will perform basic level of completeness checks on eligibility and will not be liable for incomplete submissions. NRF reserves the right to reject submissions without further review, including but not limited to, the following reasons:
 - Duplicates of proposal submitted to any other public funding agencies for simultaneous consideration
 - Missing or wrong version of Application Form
 - Inappropriate format (e.g. small font size and tight para spacing) or incomplete applications (e.g. sections left blank, missing CVs, etc.)
 - Late submission or endorsement on IGMS by the respective Director of Research
 - · Revisions made after closing date
 - Proposal not within scope of AI4S (Appendix D)
 - Ineligibility of Co-Lead PI(s) and/or Team PI(s)
 - Single investigator-led proposals
- 10.2 Please refer to **Appendix F** for Frequently Asked Questions on the Al4S scheme.
- 10.3 Additional attachments are provided for reference. Please refer to **Attachment 4** for **IGMS Application Guide** for a quick guidance on the IGMS application process.

11 Contact Information

- 11.1 For further enquiries related to the Al4S, please contact the Al4S secretariat at NRF_Al4S@nrf.gov.sg.
- 11.2 For technical enquiries related to IGMS, please contact the Helpdesk at Helpdesk@researchgrant.gov.sg.

Enclosed for Reference

- a) Attachment 1: Al4S Catalytic Call Application Form for Stage 1
- b) Attachment 2: AI4S Catalytic Call Presentation Slides Template
- c) Attachment 3: AI4S Catalytic Call Full Proposal Template
- d) Attachment 4: IGMS Application Guide

Overview of the Review Process and Requirements

8 Weeks	4 Weeks	3-4 Weeks	10 Weeks	3-4 weeks	
Launch: Call for Proposals [20 Aug to 14 Oct]	Review of Proposal Materials	Stage 1 Evaluation & Shortlisting	Stage 2 Review of Proposal Materials	Stage 2 Evaluation & Interviews	Recommendation Outcome
Opening of Online Application Form Submission Portal	Close of Online Application Form Submission Portal	Stage 1 Shortlist for Stage 2 Reviews	Evaluation of Proposal Materials	Scheduling of in-person interviews	Total time from Review of Proposals to Final
Applicants must register for an account and fill in all required fields	Completeness Check	Reviews		r Interviews	Selection: ~22 weeks
Research Proposal Materials to be uploaded: 1) Video (up to 12 minutes) 2) Proposal Slides (10- slides) 3) Full Proposal (up to 15 pages) 4) Annex to Full Proposal 5) CVs of Co-Lead Pls, Team Pl(s), Collaborators	Evaluation of Proposal Materials				

Pointers for AI for Science (AI4S) Catalytic Proposals

Articulating a 'Transformative Step-Change'

The AI4S Catalytic scheme seeks to support cutting-edge basic science proposals, that will advance the development of AI methods and tools for scientific research, and leverage these AI solutions to make a transformative step-change in scientific discovery.

A transformative step-change includes but is not limited to: i) accelerating the time taken for scientific discovery (e.g. by two-orders of magnitude (100x) or greater); or ii) enabling significantly larger or more complex hypothesis spaces to be explored; or iii) enabling scientific discoveries which would otherwise be prohibitively difficult or impossible.

The following pointers are provided for articulating how the proposed research supports transformative step-change:

- Explain how the proposed research will:
 - a) Advance the development of AI method(s) and tool(s) for scientific discovery.
 - What are the specific algorithms and approaches that will be used? Will they involve a human/expert in the loop?
 - What datasets, amount and quality of data are required, what will be required to access, obtain and/or curate the data?
 - What are the elements of novelty/significant advancement of the AI method beyond the existing state of the art?
 - b) Demonstrate the viability of these solution(s), using relevant benchmarks (e.g. ability of the solution(s) to replicate known discoveries or predictions which have been validated).
 - Set specific milestones to demonstrate that the AI-driven approach can replicate known discoveries or predictions, and benchmark them against conventional approaches (or existing AI-driven approaches).
 - Benchmarking metrics could be in terms of acceleration (e.g. time taken in days-weeks vs months-years per loop/in total time), or coverage of a significant larger hypothesis space (e.g. order(s) of magnitude larger parameter space, that includes known discoveries and extends beyond them).

- c) Leverage these solutions to make a new scientific discovery, or solve a significant problem.
 - Set specific milestones (at mid-term, completion) for new discoveries or predictions, with quantitative parameters for validation.
 - Highlight the significance of new discoveries or predictions, and the problems they would address.
- d) Extend the approach to make further scientific discoveries, demonstrating the capability to enable improvement or acceleration in the scientific discovery process.
 - Set specific milestones (at mid-term, completion) for further discoveries or predictions, with quantitative parameters for validation.
 - These targets if achieved should further highlight the viability of the Aldriven approach, its competitiveness vs the state of the art.
- Describe how the proposed work will impact one or more stage(s) of the overall scientific discovery process. Some examples of such stages, and how AI could result in a transformative step-change are provided below.
- Explain how the proposed AI solutions will accelerate or improve upon existing/baseline processes in quantitative (such as no. of trials per month, loops per day, reduction in total time, etc) or qualitative terms.
- Clearly articulate i) what datasets will be required, ii) whether the project team has
 access to such datasets, and the source of the data, if it exists, iii) what will be
 required to obtain and/or curate the datasets, if a suitable available source does
 not exist.

<u>Examples of AI for Science Impact</u> <u>on Scientific Discovery Stages</u>

Stage: 'Observation'

Examples include:

- Use of AI to identify and assess importance of features and recognise identify patterns from scientific data.
- Adapting AI models, leveraging existing knowledge in one domain, to assess feature importance/identify patterns across different domains of scientific data.

In Physics/ Earth and Climate Sciences

Discovery of patterns across multiple length and/or time scales, prediction of tipping points in complex phenomena.

In Chemistry/Materials Science

Pattern recognition to identify best performance characteristics of catalysts/materials

In Health and Biomedical Science

Discovery of genetic, phenotypic, and other diagnostic markers associated with diseases or molecular pathways of relevance to biological functions.

Stage: 'Inference'

Examples include:

- Use of AI models to infer underlying physical laws and emergent behavior from data, without explicit programming.
- Understanding the phenomenon of how neural networks exhibit prime conditions for learning, to enhance the explainability of neural networks for scientific discovery.

In Multiple Domains

Literature-based discovery to generate scientific hypotheses for further validation.

In Chemistry / Materials Science

Inferring the underlying mechanisms of and factors influencing chemical reactions, from reaction data analysis.

In Health and Biomedical Science

Deriving insights into biological processes and disease progression from patient data.

Stage: 'Prediction / Design'

Examples include:

- Building foundation models, or embedding AI models with physics / domain-specific rules to align predictions with known scientific principles.
- Utilising AI capabilities for rational design / inverse design of molecules and materials with desired properties.

In Physics/Earth and Climate Sciences Incorporating fluid dynamics/physics inspired neural networks into weather and

Stage: 'Validation'

Examples include:

- Automating research processes using Al and/or robotics to accelerate experimental validation, data collection, and analysis.
- Integrating other stages into an active learning framework, that utilises few/zero shot learning and/or optimisation and validation, to form a closed research loop.

In Multiple Domains

climate prediction models for more accurate predictions.

In Chemistry / Materials Science / Biomedical Sciences

Rational or inverse design of advanced materials, catalysts, chemicals, RNA/peptides, candidate drug molecules with desired properties.

In Health and Biomedical Sciences

Predicting onset of disease from clinical/digital phenotyping profiles of patients, predicting pharmaceutical and other interventions that restore health/biological functions.

Self-driving labs with high-throughput experimental capabilities, that can iteratively refine hypotheses, adapt experimental protocols, and navigate the vast experimental space more efficiently than traditional methods.

Do note that these stages are not prescriptive, and are intended to provide a framework for conceptualising and articulating a transformative step-change in scientific discovery. The AI4S Catalytic Grant Call welcomes proposals with potential to leverage AI in unprecedented ways, to disrupt traditional models of scientific discovery.

General Pointers for Writing Good Proposals

Good ideas are often undermined by missteps in proposal preparation. Most winning proposals have been polished repeatedly. Allow time to write and rewrite the proposal. Read the instructions and understand the evaluation criteria. Touch all the bases, and not just the ones you are comfortable with. Each section of the forms must be filled up carefully, as evaluations are based on how well the guiding questions are answered. Don't make work for the reviewers. Make it easy for the reviewers to get to your main points.

Pay heed to these general pointers:

- i) Define the problem statement and build a compelling case for need upfront. However, please do not dedicate too much time/space on prosaic background information. Elaborate more on important experimental details.
- ii) Use clear, accessible language. Avoid insider jargon and acronyms. Use direct statement and active voice.
- iii) Different parts of the projects need to be pulled together. Explain the basis for each sub-project and their linkages in fulfilling the overall programme objectives.
- iv) Show that you have an understanding of the existing competition. This should include performing a competitive scan and comprehensive literature search of ongoing efforts in the proposed topics and having an awareness of existing products/solutions or developments by the industry.
- v) Do not inflate the budget. Ask for a budget that realistically reflects the scope of work that will be accomplished. Where possible, existing equipment/facilities should be leveraged.
- vi) Clearly articulate the impact of your research and how you would achieve it. This should not be confused with KPI outputs (e.g. no. of paper publications, no. of postdocs recruited etc.). Be specific and quantitative with benchmarked technical specifications, if possible.
- vii) Root out inconsistencies in format, typos, misspellings, mislabelling of diagrams, grammar, etc. Get another person to proof-read.

Heilmeier's Catechism for Full Proposal Development

When writing your Full Proposals, try to answer these questions adapted from Heilmeier's Catechism:

- 1. What are you trying to do? Articulate your objectives using absolutely no jargon. What is the problem? Why is it hard?
- 2. How is it done today, and what are the limits of current practice?
- 3. What's new in your approach and why do you think it will be successful?
- 4. Who cares?
- 5. If you're successful, what difference will it make? What impact (esp. economical & societal) will the success have?
- 6. What are the risks and the payoffs?
- 7. How much will it cost?
- 8. How long will it take?
- 9. What are the midterm and final "exams" to check for success? How will success be measured?
- 10. Other components of proposal to be highlighted, e.g. synergies of projects within proposed programme, team composition, collaboration with academia/industry, programme management (e.g. Gantt chart, project involvement structure), relevance to Singapore etc.

Format of Curriculum Vitae

NOTE: You may also download this as a template under *Research Team, Collaborators, Referees* section of the IGMS application.

<u>For Co-Lead PI and Team PIs</u>: Please upload each CV using the format described below, as individual attachments under the *Research Team, Collaborators, Referees* section of the IGMS application.

<u>For Collaborators</u>: Please upload the CVs either under *Research Proposal* section or *Other Attachments* section of the IGMS application.

The CVs of all members (Co-Lead PI, all Team PIs and Collaborators) listed on the cover page must be provided. Each CV must start on a fresh page and be limited to 2 pages (Arial font size 12, single line spacing). Please indicate "N.A." beside the label field if the required information is not applicable. NRF will not be responsible for any missing information not provided in the CVs. Please note to only provide information listed below. Do not include any additional fields or extraneous information.

- Name
- Title
- Office mailing address
- Email
- Contact number
- Current position (please provide full details, e.g. primary appointment, joint appointments; other academic appointments including those outside of Singapore).
- Percentage of time spent in Singapore every year for the current position (mandatory field for Co-Lead PI and Team PIs)
- Employment history
- Academic qualifications (indicate institution's name and year degree awarded)
- Research interests
- List of <u>up to 5</u> (maximum) most relevant publications (including 'in-press' publications, regardless of acceptance/published date of the publications) [include authors, full title, journal name, volume, issue, page numbers]
- Patents held (related or unrelated to the study), and/or Scientific Awards, if any.

CHECKLIST FOR PREPARATION OF A RESEARCH BUDGET

Before you Begin

- 1. Read NRF's Instructions for Submission of Full Proposal for the Al-for-Science (Al4S) funding scheme carefully.
- 2. Review the instructions and guidelines to ensure that the proposed items are eligible and in concordance with your Host Institution's policies.
- 3. When in doubt, always seek assistance from your Office of Research or NRF before you begin.

Preparing the Budget

- 4. Be realistic and do not over-inflate the budget. Budget should be reasonable and appropriate for the proposed research plan. For multi-year projects, consider time constraints and get advice on whether you will be able to spend the proposed budget within the duration of the project.
- 5. Be detailed and specific. List all items on a separate worksheet that clearly shows the calculations and keep this detailed list to remind yourself how the numbers were derived. This will be useful during the budget scrubbing stage (prior to award) and for future monitoring and reporting.
- 6. Anticipate reviewers' views and plan ahead to ensure that detailed description and justification on the need of all items listed in the budget are written clearly.
- 7. Direct costs refer to costs which can be directly attributed to the project. Indirect costs are Institution overhead costs that benefit and support research.
- 8. Please use the checklist below to assist you with preparation of the research budget.

S/N	Item	Description	
1.	Manpower Cost (EOM)	· · · · · · · · · · · · · · · · · · ·	
2.		Is the proposed manpower headcount sufficient and reasonable to meet the project objectives and deliverables?	
3.		Is the EOM per pax in agreement with the salary package stipulated by your Host Institution's HR policy?	
4.		Have you budgeted the EOM according to the man- months required of each manpower headcount within the project duration?	
5.		Have you budgeted for the residency requirements for the international team members (if any)?	
6.		Have you sufficiently justified the role for each manpower headcount and the need to recruit him/her to meet the project objectives?	
7.	Equipment	Have you explored alternative sources for using existing equipment without the need to purchase new equipment?	
8.		Can you use the equipment in shared facilities and utilise AI4S fund to pay for service fees instead?	
9.		Do you have sufficient space for the new equipment? What is the usage frequency of the new equipment? Does the equipment require high maintenance cost?	
10.		Have you factored in taxes, exchange rate (if applicable) and freight charges (if applicable) for the proposed equipment item?	
11.	Consumables Costs (OOE)	Have you listed all the supplies and materials required?	
12.		Have you considered the cost associated with use and access to unique, high-quality and comprehensive dataset, as well as compute?	
13.	Research Scholarship	Are the tuition fees and stipend rates budgeted according to the MOE prevailing rates?	
14.	Overall Budget	Does the amount of all line items of each vote tally?	
15.	Daagot	Does the total amount of all votes tally with the final proposed budget?	

I. AREAS OUT OF AI4S SCOPE

The AI4S Scheme is not intended for the following areas:

- a) Epidemiological and behavioural studies;
- b) Observational studies (including cohort, longitudinal, case-control studies, etc.);
- c) Clinical and drug trials;
- d) Health services research/operations research;
- e) Infrastructure/facilities set-up; and
- f) Market/drugs/product development.
- g) Incremental research in domain and/or Al fields

II. NON-FUNDABLE DIRECT COSTS

Types of Expenses	Description
Salaries ⁵ of Co-Lead PI / Investigators / Project Leads	Not allowable, to ensure no double funding of salaries and related costs, as the salaries are already supported from other sources (e.g. faculty salaries are supported separately by the IHLs as it is in support of the IHLs' core mission).
Salaries of Teaching staff / Teaching substitutes	Not allowable, as this is being supported from capitation grants.
Undergraduate tuition support	Not allowable, as this should be supported under the respective scholarship grants and bursary schemes.
Salaries of general administrative staff	Not allowable, as this is an indirect cost*.
Costs related to general administration and management	Not allowable, as this is an indirect cost*. This includes common office equipment, such as furniture and fittings, office software, photocopiers, scanners and office supplies.
Costs of office or laboratory space	Not allowable, as this is an indirect cost*. This includes renovation/outfitting costs, rent, depreciation of buildings and equipment, and related expenditures such as water, electricity, general waste disposal and building/facilities maintenance charges.

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Residency of international PI(s) in Singapore may be budgeted for in the proposal and will be supportable by the grant. Eligible items for residency include travel, accommodation, and cost of living allowance (to cover meals, transport, incidentals). Salary of international PI(s) will not be supportable under the AI4S Catalytic Grant.

Personal productivity tools & communication expenses	Not allowable, unless the use of mobile phones and other form of smart devices were indicated in the methodology for the Research. All other cost under this expense type is an indirect cost*.
Entertainment	Not allowable, as this is an indirect cost*.
Refreshment	Not allowable, unless this is related to a hosted conference or workshop for the Research. All other cost under this expense type is an indirect cost*.
Audit fees (Internal and external audit) and Legal fees Fines and Penalties Professional Membership Fees Staff retreat and team-building activities	Not allowable, as this is an indirect cost*.
Patent Application	Not allowable, as this should be supported from overheads given to I&E Office (IEO)*. This includes patent application filing, maintenance and other related cost.

^{*}Note: Indirect costs should be funded from overheads or other funding sources.

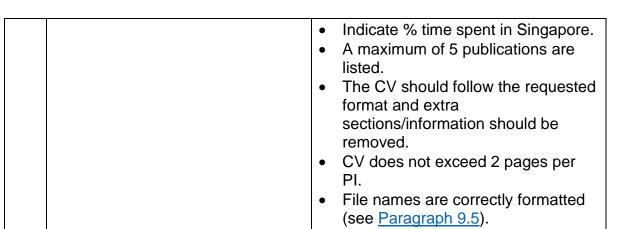
APPENDIX E

GUIDING CHECKLIST FOR AI-FOR-SCIENCE (AI4S) COMPLETENESS CHECKS

This is a non-exhaustive list for PIs to take reference to ensure completeness of the submissions, and for the Office of Research to take reference when verifying the submissions.

S/N	Document	Section	Item to Check
1	Application Form for Stage 1	Overall	 Co-Lead and Team Pls fulfil the eligibility criteria. NRF will defer to the institution's assessment on whether Co-Lead Pls and Team Pls are qualified. Proposal fits the Al4S scope.
2		Section II: Main Stage 1 contents (Video)	 Link to Video has been inserted into the application form. Video Link is functional, accessible, downloadable; and does not exceed 12 minutes. Video does not exceed 500MB. Video contains relevant information (research objectives, competitive scan, approach, outcomes & deliverables) Application Form is maintained in Word Format to keep hyperlinks
3		Section III: Declaration by Grant Applications	 The Co-Lead Pls, all Team Pls and Collaborators (if any) have signed the document. The dates of signatures fall within the grant call launch period.
4	Presentation Slides	Presentation Slides	 Presentation Slide Cover Page contains Proposal ID, title, budget (with direct costs) that match with the IGMS online application. Includes ORCID for Co-Lead and Team PIs Presentation Slides contain all relevant sections (research objectives, assessment on current development, proposed approach, outcomes, and deliverables) and are within the 10-slides limit (excluding Cover Page).

5	Full Proposal	Section I: Cover Page	 Presentation slides are in pdf format (no larger than 4 MB) and must be uploaded into Research Proposal Section of IGMS. Presentation slides use at least Arial font size 12 for all text and figures. Proposal ID, title, budget (with direct costs) match with the IGMS online application. Includes ORCID for Co-Lead and Team Pls.
		Section II: Research Proposal	 Full Proposal is within 15-page limit. All sub-sections (research objectives, assessment on current development, proposed approach, programme plan, role of team members, outcomes from previous grants, and outcomes and deliverables) are addressed and are within the 15-page limit. This section in written in Arial font size 12, single spacing, normal margins.
6	Annex to Full P	roposal	 The Annex is a continuous document uploaded as a single file. Headings are used for each subsection. Full titles, DOI numbers are included for all references. Ensure that all mandatory sections in the Annexes are provided File Names are correct (see Paragraph 9.5). For optional section, only figures, charts, diagrams or tables are allowed with clearly labelled headings and appropriately referenced in the Application Form for Stage 1 or Full Proposal respectively.
7	CVs		All team members (Co-Lead PIs, Team PIs and collaborators) should each provide a CV.



APPENDIX F

Frequently Asked Questions

General

S/N	Question	Response			
Appl	Application				
1	What is "use-inspired basic research"?	The research undertaken is inspired by the quest to advance fundamental scientific knowledge and understanding that is motivated by an unmet need or to address a practical problem. The research need not necessarily lead to immediate translation or commercialisation within the duration of the project.			
2	Does Al4S fund blue-sky or curiosity-driven research?	Al4S Catalytic scheme supports transformative use- inspired research. The scheme is aimed at stimulating new collaborations between domain and Al researchers, to create a large base of activity in Al for research.			
3	How important is industrial participation for the different AI4S categories? Is it mandatory to include industrial partner(s)?	Industry partnership is not a requirement for AI4S. It is not mandatory to include industrial partner(s). If industrial partner(s) are involved, they should provide letters of support with details of their contribution and/or commitment to the project.			
4	Is stakeholder agency consultation required prior to submission?	This is not a mandatory requirement.			
5	Can a PI submit multiple proposals under the same AI4S category as the Co-Lead PI at the same time?	Yes, if the proposals are substantially different and there are no overlaps in the scope of the work to be funded.			
6	Can the Co-Lead and Team PI(s) be from the same group?	Yes.			
7	If a PI has submitted a proposal in another funding scheme which is pending review, can he/she still apply for AI4S?	The PI should not submit the same proposal (which is pending review in another funding scheme) to Al4S. He/she can submit a different proposal (with no overlaps in scope) to Al4S.			
8	Can the Al4S scheme accept proposals with humanities or social sciences elements?	Yes, humanities and social sciences elements can be included in the proposals. However, the proposals should have a STEM (Science, Technology, Engineering, Mathematics) focus.			
Eligi	bility Criteria				
10	Are early career scientists (e.g. post-docs) eligible to be Lead or Team PIs? How do we determine if a PI meets the criteria of a Lead or Team PI?	We will leave it to the Institutions to endorse your qualification as either a Co-Lead or Team PI, as there are institutional differences in designations, ranks, roles and responsibilities. Institutions should read the Eligibility Criteria and ensure applicants meet the requirements.			
11	Can a Co-Lead or Team PI come from overseas?	No. International PIs who do not fulfil eligibility criteria to participate as Co-Lead or Team PI can participate as Collaborators.			

Asse	Assessment				
12	What is the expected TRL of AI4S projects at completion?	The Al4S scheme supports transformative use inspired basic research.			
13	What are the outcomes or Key Performance Indicators (KPIs) expected of AI4S projects?	Al4S projects will be assessed on the extent they have achieved their scientific deliverables (stated in their proposal), how they have advanced fundamental scientific knowledge, accelerated scientific discovery and facilitated transformative research outcomes.			
		A good metric of successful research outcomes is the continuity of the research, and whether teams go on to secure larger grant funding, or contribute to establishing peaks of research excellence in Singapore.			
		As part of annual progress reports, NRF may request projects to report indicators such as publications, technical disclosures or patents etc for tracking purposes, but projects are <u>not</u> expected to provide targets for these indicators and will not be assessed solely based on these.			
14	What kind of feedback will be given for non-shortlisted proposals?	A comprehensive reviewer report will be provided for reference, for each non-shortlisted proposal. For proposals that are rejected without review, NRF will provide reasons for rejection (e.g. if the proposed research falls outside the scope of the grant call).			
Bud	get				
15	Can international collaborators receive funding for some elements of the research?	Applicants may propose OOE budget lines for Visiting Professors/Experts, which can cover honorarium, travel and accommodation expenses. Visiting Professors/Experts should be clearly identified in the proposal, or to NRF, with justifications for visits provided.			
16	Does all the funding have to be spent within Singapore?	RIE funding is intended to fund research activity conducted by the Team (Co-Lead PIs and Team PIs) within Singapore.			
		Applicants may propose budget items under Overseas travel, e.g. attending overseas conferences or to access equipment/facilities overseas with justifications provided, excluding the conduct of R&D activity.			
17	Can the AI4S Catalytic grant support: a) Salaries of Co-Lead and Team PIs? b) Hiring of management support officers (MSO)? c) Hiring of Project/Programme Manager? d) Subscription of GPU and cloud services?	 (a) No. (b) No. It does not support salaries of administrative staff, including MSOs. (c) Yes, if the Programme Manager's role is related to the Research, and not purely administrative. (d) Yes, applicants may propose OOE budget lines to support facilities usage, and subscription of services such as GPU and cloud usage. Please refer to the list of nun-fundable direct costs in the Guidelines for the Management of Research Grants that is issued to the Heat Institutions. 			
18	Do all AI4S categories provide indirect costs?	Yes, the indirect cost is 15% of the direct cost, with exception for research scholarship.			

Area	Areas out of scope for AI4S				
19	It is stated in the Grant Call information sheet that AI4S is not intended to support research in the following areas:	Proposals with a research focus in the areas listed should be submitted to other more appropriate funding schemes in Singapore, for funding consideration.			
	(i) epidemiological and behavioural studies; (ii) observational studies (including cohort, longitudinal, case-control studies, etc.); (iii) clinical and drug trials; (iv) health services research/operations research; (v) infrastructure/facilities set-up; and (vi) market/drugs/product development (vii) incremental research in domain and/or AI fields Can elements of the above be incorporated in AI4S proposals?	Al4S proposals should be primarily driven by basic scientific discovery and advancement of scientific knowledge that is use-inspired, and should have a STEM (Science, Technology, Engineering, Mathematics) focus. Some elements of research in the areas listed can still be incorporated in Al4S proposals but should not form the sole or main objectives of the proposal, and their inclusion will need to be well justified.			
Oth	ers	1			
20	Where can the list of past awarded projects be found?	A list of awarded projects would be published on the NRF website.			

AI4S Application

S/N	Question	Response
21	Is AI4S intended to only fund large scale programmes?	The Al4S Catalytic scheme will provide funding support for programmes up to a period of 3 years.
23	Is there any action required from the team if a proposal is shortlisted for interview?	Teams would be informed if their proposals are invited for in-person interview at the Evaluation Panel meeting.
24	How much preliminary data is expected for a Al4S proposal?	Inclusion of preliminary data is encouraged but is not mandatory for an AI4S proposal submission. The proposal should still clearly articulate i) what datasets will be required for the proposed advancement and use of AI methods and tools for scientific discovery, ii) whether the project team has access to such datasets, and the source of the data, if it exists, iii) what will be required to obtain and/or curate the datasets, if a suitable available source does not exist.
25	How will AI4S proposals be reviewed? Will there be nominated external reviewers?	Al4S proposals will be reviewed by an Al4S Evaluation Panel comprised of international researchers/ academics. Reviews may be supplemented by independent reviewers who possess relevant subject-matter expertise.