**AI SINGAPORE RESEARCH PROGRAMME**

**PROPOSAL APPLICATION FORM**

**All information is treated in confidence. The information is furnished to AI Singapore with the understanding that it shall be used or disclosed for evaluation, reference and reporting purposes.**

**SECTION 1: Cover Page *(All fields are mandatory)***

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| **Proposal Title: XX (Bold, Font 11)** | | |
| **Grand Total** **Cost** (Direct + Indirect Research[[1]](#footnote-1), including Research Scholarship if applicable): **S$ XX** | **Period of Support: XX years** | **Host Institution** *(please indicate only one host)****:* XX** |
| **Vision of the Proposal** *(Select the vision applicable to your proposal. See Annex D for descriptions)***:**  **Discriminating Information**  **Towards Human Omnitasking**  **Removing Unwanted Digital Footprints**  **AI for Science** | | |
| **Research Topics of the Proposal** *(Select the proposal’s chosen research topic(s) to enable the vision. See Annex D for descriptions)***:**   |  |  | | --- | --- | | **Discriminating Information** | **Towards Human Omnitasking** | | Information authentication, bias, benchmarks, and evaluation  Interpretation and generation  Assessment of impact and user profiling | Multimodal understanding and summarization / Conversational NLP  Cognitive state tracking / Commonsense reasoning  Behavior understanding / Personalization  Trustworthy and explainable AI / Human-AI collaboration | | **Removing Unwanted Digital Footprints** | **AI for Science** | | Definition of unwanted footprints  Footprint removal algorithms  Footprint removal auditing  Evaluation of organizational trustworthiness | AI for natural law extraction and understanding  Foundational AI models for fast, accurate, large-scale scientific discovery  AI for inverse design in science  AI that maximizes a priori knowledge  AI for data-sparse science  Learning representations for scientific creativity  AI for quantum science | | | |

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| **Classification of AI Core Technical Areas of the Proposal (select a maximum of 3 only):**   |  |  | | --- | --- | | **Cognitive modelling and systems**  **Game theory and economic paradigms**  **Heuristic search and optimization**  **Knowledge representation and reasoning**  **Machine learning**  **Multiagent systems** | **Natural language processing (NLP)**  **Planning and scheduling**  **Reasoning under uncertainty**  **Robotics**  **Search and constraint satisfaction**  **Vision** | |

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| **Project Team Members** *(Please add/delete rows where necessary)* | | | | | | |
| **Role** | **Name** | **Google Scholar or DBLP**  **iD[[2]](#footnote-2)** | **Designation** | **Department/ Institution** | **% effort within project[[3]](#footnote-3)** | **% of time committed on the project[[4]](#footnote-4)** |
| ***PI*** |  |  |  |  |  |  |
| ***Co-PI (1)*** |  |  |  |  |  |  |
| ***Collaborator (1)*** |  |  |  |  |  |  |
|  |  |  |  | **Total:** |  |  |

**SECTION 2: Details of Research Proposal**

Please ensure all fields are completed. Proposal contents should not exceed **10 pages**. Diagrams, references and Gantt chart should be attached as appendices (excluded from the page limit). **Please use Arial font size 11, single line spacing and default margins of this document.**

1. **Executive Summary:** *400 to 500 words of executive summary on the proposed project (approximately one-page, included in the page limit), written in layman terms and avoiding scientific jargons, where practicable. The headers and descriptions in executive summary should align with Research Proposal, where practicable.*
2. **Research Objectives:** *This section should articulate clearly the use-inspired objectives and expected outcomes of the project. Additionally, you must share a striking vision of the major foreseen downstream benefits of this project on society. This could be achieved through directly enabling new high-impact technologies and capabilities, or through creating the opportunity for subsequent projects to do so. This must be compelling and easily understandable to people outside the field, without use of technical jargon.*
3. **State of Current Research:***How is it done today, who are the leading researchers studying the targeted problem/objectives, and what are the limitations of their current approaches?*
4. **Proposed Approach:** *What is your approach? What is the potential for scientific breakthroughs or disruptive innovation arising from your approach? Please provide a competitive scan of existing state-of-the-art developments and compare your proposed technology/system/solution in quantitative terms. Describe previous and ongoing works, and any preliminary results, providing all necessary details that would help support this proposal. Why do you think your proposal will be successful in addressing the problem?*
5. **Project Plan:** *How are financial and human resources organised to accomplish the objective? How coherently do the sub-projects contribute and synergise towards achieving the research objectives? What are the technical risks and how would these be mitigated? Outline the schedule for all phases of the proposed programme – a Gantt chart has been provided in Annex A.*
6. **Role of team members**: *What are the roles and contributions of the Co-PIs and Collaborators? Briefly describe the plans for interaction among the team member(s) and Collaborator(s) in achieving the research objectives. What are the track records and capabilities of the PI and Co-PIs and how are their expertise relevant to the research programme? How are the Collaborator(s) augmentative and relevant to the research programme?*
7. **Outcomes & Deliverables:** *What are the scientific milestones/ metrics that can be used to appropriately measure success at periodic review and at completion of the programme against the stated research objectives? Be quantitative if possible (e.g.: a 2X improvement, or a specific achievement). Explain what impact the success of the project would be for the economy and/or society, and how it would generate value for Singapore in the field of AI technologies/capabilities.*
8. **Ethics Statement (maximum 1 page, excluded from the 10-page limit):** *Proposal submissions are expected to include a statement of the potential negative ethical/societal impacts of the proposed research. Submissions should also provide description on how these risks can be mitigated, if identified, and should not contain information that should otherwise be in the main proposal.*

**SECTION 3: Proposed Budget**

Content in sub-section ‘(3.1) Summary’ should not exceed 1 page. The amount requested for each budget line item must be documented and justified in sub-section ‘(3.2) Detailed Breakdown & Justifications’.

* 1. **Summary**

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| --- | --- |
| **Budget Category** | **Budget(S$)** |
| **Expenditure on Manpower (EOM)** |  |
| 1. **Expenditure on New Equipment (EQP)** |  |
| 1. **Other Operating Expenses (OOE)** |  |
| 1. **Overseas Travel (OT)** |  |
| 1. **Research Scholarship (RS)** |  |
| **Total Direct Costs (S$):***. Formula: (EOM+EQP+OEE+OT+RS)* |  |
| **Indirect Research Costs (S$):** *Singapore-based Institutes of Higher Learning, Research Institutions and/or publicly-funded Medical Institutions selected to host AI Singapore projects will be eligible for indirect research cost (IRC) funding of up to* ***30%*** *of the direct cost approved. Research Scholarship does not invite any IRC funding. Formula: (EOM+EQP+OOE+OT)\*IRC%* |  |

* 1. **Detailed Breakdown & Justifications**

*(Please add rows where necessary)*

* + 1. **Expenditure on Manpower (EOM)**

*Projections should include salary/honorarium and costs of all other remunerative benefits (e.g. employer cpf, etc)*

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| **Item No.** | **Description** | **Unit Rate per Man-Month**  **(S$/month)** | **# of Man-months**  **(Month)** | **Sub-total (S$)** | **Justification** |
| EOM01 | *Research Fellow 1* |  |  |  |  |
| EOM02 | *Research Fellow 2* |  |  |  |  |
| EOM03 | *Research Associate 1* |  |  |  |  |
| EOM04 | *Research Assistant 1* |  |  |  |  |
| EOM05 | *Student Intern 1* |  |  |  |  |
| EOM06 | *Please add or delete rows, where necessary* |  |  |  |  |
| **EOM Total:** | | | |  |  |

* + 1. **Equipment (EQP)**

*Please include GST, where applicable. Written quotations should be appended for equipment with value >$100,000 requested. State whether similar equipment exists in the PI’s/Co-PIs’ labs or department/school. If so, justify why a new equipment is required for the project*

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| **Item No.** | **Description of Equipment** | **Cost Per Unit (S$)** | **# of Units** | **Sub-total**  **(S$)** | **Justification** |
| EQP01 |  |  |  |  |  |
| EQP02 |  |  |  |  |  |
| EQP03 |  |  |  |  |  |
| EQP04 |  |  |  |  |  |
| EQP05 | *Please add or delete rows, where necessary* |  |  |  |  |
| **EQP Total:** | | | |  |  |

* + 1. **Other Operating Expenses (OOE)**

*Please include GST, where applicable.*

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| **Item No.** | **Description of Expenses** | **Cost per Unit**  **(S$)** | **# of Units** | **Sub-total**  **(S$)** | **Justification** |
| OOE01 |  |  |  |  |  |
| OOE02 |  |  |  |  |  |
| OOE03 |  |  |  |  |  |
| OOE04 | *Please add or delete rows, where necessary* |  |  |  |  |
| **OOE Total:** | | | |  |  |

* + 1. **Overseas Travel (OT)**

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| **Item No.** | **Description of Trip** | **Cost per Trip**  **(S$/Trip)** | **# of Trips** | **Sub-total**  **(S$)** | **Justification** |
| OT01 |  |  |  |  |  |
| OT02 | *Please add or delete rows, where necessary* |  |  |  |  |
| **OT Total:** | | | |  |  |

* + 1. **Research Scholarship (RS)**

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| **Item No.** | **Description of Scholarship Support** | **Cost per Year**  **(S$/Year)** | **# of Year** | **Sub-total**  **(S$)** | **Justification** |
| RS01 |  |  |  |  |  |
| RS02 | *Please add or delete rows, where necessary* |  |  |  |  |
| **RS Total:** | | | |  |  |

**SECTION 4: Declaration of Other Funding Support**

* 1. **All Grants Currently Held or Being Applied**

Please provide details (all fields are mandatory) for all currently held or applied grants by the PI and all Co-PIs listed on the cover page (not required for Collaborators). These include those **supported by and/or applied** to universities, other public funding agencies and foundations. Please indicate “N.A.” for any PI/Co-PI with currently no awarded grants or grants being applied for. Note that all PI and Co-PIs must be accounted for under this section.

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| **S/N** | **Title of Supported Project** | **Funding Agency** | **Status (Awarded/ Applied)** | **Total Amount Awarded/ Applied for (S$)** | **Years of Support** | **Grant End Date (dd/mm/yyyy)** | **Granted to Who** |
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If any of the currently held grants above fund research topics related to the AI Singapore proposal, please include **a one-page supplementary write-up as an annex** (Template found in Annex C). The one-page supplementary write-up is to describe the research funded by these grants, and how the objective and research differ from that in the AI Singapore proposal.

* 1. **All Other Funding Support**

Please provide details on the funding or other resources to be provided by any participating industry/institute partner(s) for the applied grant.

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| **Type of Funding**  *(please indicate In-Kind or Cash)* | **Funding Organisation** | **Duration of Support**  **(No. of Years)** | **Expiry Date (dd/mm/yyyy)** | **Funding Amount**  **($S)** |
| *Please add or delete rows, where necessary* |  |  |  |  |
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| **Total Amount:** | | | |  |

**SECTION 5: Performance Indicators**

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| **Key Performance Indicators** | | **Target number to be**  **Achieved at the end**  **of Project** | **List the Conferences and Journals for submission of papers** |
| 1**.** | **No. of Top 10% Publications**  *(Total number of journal papers and conference papers/presentations published)* |  | *(e.g. AAAI, NeurIPS)* |

**SECTION 6: Names of Suggested International Reviewers**

PIs must nominate **at least three (3)** international peer reviewers.

Reviewers should be **active AI** **experts** in the field who are able to provide an independent and credible assessment of the research proposal.

* In general, reviewers should be at least Assistant Professors or equivalent. Doctoral students should not be nominated as reviewers.
* PI should suggest names of people whom are likely to serve as reviewers.
* Nominees, who have moved to other research fields or have moved into administration and left research altogether are not good candidates.
* Additionally, very senior figures in the field are not good candidates due to high volume of duties and obligations.

PIs should disclose their relationship and past collaborations with the reviewers, if any.

The Scientific Evaluation Committee may choose not to engage the suggested reviewers.

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| **S/N** | **Name of Reviewer** | **Institution** | **Designation** | **E-mail address** | **Research interest / Expertise** | **Relationship to PI/Co-PI** |
| **1** |  |  |  |  |  |  |
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**Section 7: Declaration by Grant Applicants**

In signing this grant application, the PI and Co-PI(s) UNDERTAKE, on any grant award to:

* ensure that all PI and Co-PI(s) meet the listed eligibility criteria;
* ensure that a proposal with similar research aims has not been sent for and/or awarded research funding either by AI Singapore, NRF or another funding agency;
* be actively engaged in the execution of the research;
* ensure that AI Singapore and NRF are acknowledged in all publications and/or research outcomes;
* ensure that a copy of all publications arising from research wholly or partly funded from this Scheme will be submitted to AI Singapore;
* comply with the provisions of any relevant laws of the republic of Singapore, statutes, regulations, by-laws, rules, guidelines and requirements applicable to it, as well as all applicable policies and procedures adopted by AI Singapore and/or NRF as the same may be amended or varied from time to time; and
* agree to hold primary responsibility for the responsible conduct of research, and shall abide and comply with the ethical, legal and professional standards relevant to research, in accordance to the research integrity policy of the Host Institution.

We declare that the facts stated in this application and the accompanying information are true. This is an original and latest version of the proposal. We also declare that no other versions of this proposal (or parts thereof) with similar objectives, scope, deliverables or outcomes have been or will be submitted to any other funding bodies.

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| **Name of Applicant** | **Signature** | **Date Signed** |
| Principal Investigator  <Name of Applicant> |  |  |
| Co-Principal Investigator (1)  <Name of Applicant> |  |  |
| Co-Principal Investigator (2)  <Name of Applicant> |  |  |
| Co-Principal Investigator (3)  <Name of Applicant> |  |  |
| Co-Principal Investigator (4)  <Name of Applicant> |  |  |

*Please add rows if necessary.*

**Section 8: Endorsement by the Host Institution**

In signing the grant application, the Host University UNDERTAKES, on any grant award, to:

* + ensure that the Principal Investigator (PI) meets the defined eligibility criteria;
  + provide appropriate support during the grant period;
  + ensure that the funds provided are used for the appropriate purposes and managed according to the terms and conditions stipulated in the Letter of Award; and
  + ensure that all budget requests are in accordance with the IHL/RI’s prevailing policies and financial guidelines.

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| **Proposal Title** |  |
| **Lead PI** | (Capitalised FAMILY NAME) |

Comments:

Name and Signature of Director of Research (or equivalent) / Date

**ANNEX: Checklist**

Please attach the following annexes in pdf format, under *Research Proposal* Appendices section:

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| **Item** | **Remarks** | **Description** |
| **Annex A** | Mandatory for all applications | A project implementation schedule to outline the plans for the proposal. |
| **Annex B** | Mandatory for all applications | Copies of all applicants’ CVs in the proposed format. Letters of Commitment: letters from all collaborators (if any) to state their role and contribution to the research. |
| **Annex C** | Mandatory if the AISG Research Grant 2022 application is related to currently held grant(s). | Describe the research funded by currently held grant(s), and how the objective and research differ from that in the CRP application.  Refer to Section 4: Declaration of Other Funding Support |

**ANNEX A: Project Implementation Schedule**

The proposed schedule will be used for assessment and evaluation of the project. A satisfactory progress is required for continued disbursements of funds and will also be taken into consideration for future AI Singapore grant application and for grant renewal. Projects are expected to commence operation no later than two months from the start date of the project.

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| **Quarters**  **Project Implementation Schedule** | **Year 1** | | | | **Year 2** | | | | **Year 3** | | | | **Year 4** | | | | **Year 5** | | | |
| **Q1** | **Q2** | **Q3** | **Q4** | **Q4** | **Q2** | **Q3** | **Q4** | **Q1** | **Q2** | **Q3** | **Q4** | **Q1** | **Q2** | **Q3** | **Q4** | **Q1** | **Q2** | **Q3** | **Q4** |
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**ANNEX B: Curriculum Vitae**

Please note the eligibility requirements:

1. PIs and Co-PIs from publicly-funded Institutes of Higher Learning (IHLs)[[5]](#footnote-5) and Research Institutions (RIs)[[6]](#footnote-6) in Singapore are eligible to participate in the call. Private sector and other entities can participate as Collaborators.
2. PI must fulfil the following requirements:

* Hold a primary appointment (i.e. a minimum time commitment of 9 months per year in Singapore) in a Singapore-based Institute of Higher Learning (IHLs) and/or Singapore-based Research Institute;
* Must be an expert in AI domain; an AI expert is defined as a person with strong track record of publications from AI conferences and journals; and
* Be an independent PI with a track record of leadership ability in coordinating research programme(s) and providing mentorship to research team(s), as well as having productive research outcomes.

1. Co-PI must fulfil the following requirements:

* Hold a primary appointment in Singapore-based Institute of Higher Learning (IHLs) or Research Institution (RI).

1. The CVs of all members (**PI, all Co-PIs and Collaborators**) listed on the cover page must be provided according to the format below. **Each CV should start on a fresh page and be limited to 2 pages.** Please indicate “N.A.” beside the label field if the required information is not applicable and note that AI Singapore will not be responsible for any missing information not provided in the CVs.

* 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, if applicable)
* Employment history
* Academic qualifications (indicate institution’s name and year degree awarded)
* Research interests
* List of 5 most significant publications (in the past 3 years only, i.e. 2020 - 2022) relevant to the proposal
* Patents held (related or unrelated to the study)
* Scientific awards

**ANNEX C: Declaration of Other Funding Support Supplementary**

Please note the eligibility requirements:

PI and Co-PIs should note that **parallel submissions are not allowed** – i.e. applicants must never send similar versions or part(s) of the current proposal application to other agencies or grants for funding (or vice versa).

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| **S/N** | The serial number should correspond with the proposal declared in Section 4 |
| **Title of Supported Project** |  |
| **Funding Agency** |  |
| **Status** |  |
| **Total Amount Awarded/ Applied for (S$)** |  |
| **Years of Support** |  |
| **Grant End Date (dd/mm/yyyy)** |  |
| **Granted to Who** |  |
| **Description** | It should cover:   1. Description of the research funded by other awarded/applied grant. 2. How the objective and research differ from the proposal submitting to AI Singapore. |

**ANNEX D: Descriptions of Proposal Visions and Enabling Research Topics**

**Discriminating Information**

Advances in technology have enabled the rapid creation and dissemination of information, for instance, via social media. This ability to quickly reach mass audiences has the potential to impact individuals and society as a whole, sometimes adversely, should misinformation or disinformation be spread. For instance, in the recent COVID-19 pandemic, misinformation about the disease, potential treatments and vaccines could have resulted in adverse impact on the health of individuals or even the population in general. As another example, deepfakes could be used for manipulation, or even cause harm, when widely disseminated. AI systems can potentially help in detecting such misinformation/disinformation and assessing its impact on individuals and society, and the focus of this theme is to develop novel methods towards these goals.

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| **Enabling research topic** | **Description** |
| Information authentication, bias, benchmarks, and evaluation | Defining disinformation: Whether a piece of communication is disinformation or not largely depends on the intention of the creator. How then can disinformation be appropriately defined for developing an AI system to discriminate it?  Multimodality/Multilinguality: How can we leverage multimodal features in media for better detection, monitoring and prevention of misinformation? How can we develop systems that can handle multiple languages?  Role of external knowledge: What is the role of external knowledge, and how can we best utilise it?  Detection vs. prevention: How can AI be used not only for detection of misinformation but also for prevention of misinformation, such as through educating the general public?  Use cases: The concrete, real-world use cases and benchmarks are urgently needed to drive the research.  Evaluation against dynamically changing information: How can AI methods handle the uncertainty of ground truth that often comes with unverified information, since the ground truth may dynamically change when the event unfolds and new information keeps coming in? |
| Interpretation and generation | Robustness of detection systems: There are attacks designed to evade misinformation/deepfake detection systems. For example, there are many possible deepfake synthesis systems and it is not feasible to collect data from all of these. So, building in robustness and fast adaptation of systems to new attacks would help mitigate spread of such harmful information.  Interpretability/explainability of detection systems: Can these systems identify specific features of the input (e.g., pixels in images or words in news text) that contain artifacts suggesting that the input has been manipulated? For example, for deepfake, this may involve identifying the pipeline of manipulations used to generate the deepfake. This would both aid detection algorithms and facilitate human-AI collaboration to better identify misinformation/deepfakes.  Source attribution: How can we design methods to identify which entity has generated the misinformation/deepfake? For misinformation propagated through online social networks, this may involve analysis of the propagation patterns in the social network graphs. Content Provenance and Authenticity. |
| Assessment of impact and user profiling | Early detection: To reduce the impact of the spread of misinformation, developing early detection methods is critical.  Impact quantification: How to quantify the impact of mis/disinformation?  Understanding of vulnerability: What makes someone vulnerable to misinformation? This may require an interdisciplinary approach with people from communication and computer science working together.  Understanding of behaviours: For some malicious misinformation such as scams, the scammers perform a series of actions to deceive users. Understanding such scammer behaviours is important for detection and prevention. |

**Towards Human Omnitasking**

Human multitasking can result in time wasted due to human context switching and becoming prone to errors due to insufficient attention. Advances in digitalization have enabled business processes to be conducted in virtual environments by leveraging human-AI collaborations. Human omnitasking is the concept that the AI technology that can split one’s attention on more than one task or activity at the same time. For example, attend online virtual conferences on the phone while driving. AI systems can also assist a human user to rapidly shift attention between the tasks and perform the tasks well or even learn the behaviour of the human user and act as an avatar to imitate the user to response to multiple tasks. Multiple avatars can be the delegate on behalf of the human user to attend multiple virtual conferences/meetings/gatherings at the same time. Are they feasible? Are they desirable? The goal is to assist human workers to be able to perform tasks more efficiently, anywhere, anytime and increase his/her productivity by a margin.

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| **Enabling research topic** | **Description** |
| Multimodal understanding and summarization / Conversational NLP | Given a particular situation and a history of what happened previously, how can AI systems optimally help a human worker “get up to speed”? For example, if a person steps out of a meeting for an urgent call, or leaves a real-time operation for a break, what should an AI assistant say, show or do, in the most economical and effective way, to help the person? |
| Cognitive state tracking / Common sense reasoning | Given a particular situation, what is a human user or worker likely to be thinking, feeling, wanting to achieve and planning to do next? In order to effectively assist a person in omnitasking, AI systems need to understand what people are experiencing and then complement them. What might the person have missed or forgotten? What do they already know and what else do they need to know or pay extra attention to? |
| Behaviour understanding / Personalization | Does a particular worker tend to make the same mistake repeatedly? Do they perform certain tasks in a sub-optimal way? Could an AI system replicate the person’s task behaviour but perform it without mistakes or more quickly? Could lapses of attention be spotted and likely mistakes pre-empted? |
| Trustworthy and explainable AI / Human-AI collaboration | For humans to rapidly and effectively interact with one or more AI agents, there needs to be a certain level of trust and understanding. How can trust be built initially and how can level of trust be gauged? Once a certain level of trust is established, what can be adjusted or re-calibrated or sacrificed to increase the level of omnitasking for greater productivity? |

**Removing Unwanted Digital Footprints**

AI systems are often trained on data collected from individuals, such as face images, medical records, and online interactions. As supported by recent privacy regulations such as GDPR, each individual has “the right to be forgotten”, i.e., she may request all digital traces about her to be removed from an AI system, to prevent others from inferring or utilizing her information. To enable such individual rights, we need to develop technologies for (i) identifying and removing unwanted digital traces from AI systems and (ii) auditing and certifying the removal of such traces in AI systems.

Societal benefits: The technologies to be developed will enhance personal privacy protection, which is much needed in the era of big data. In particular, they will enable individuals to gain better control on where and how their data could be used, thus providing supports for data privacy legislations such as PDPA and GDPR. In addition, they will improve the privacy guarantees of AI systems and help address the growing public concerns on the misuse of personal data in AI. Furthermore, they can also be applied to remove the influence of corrupted or malicious data in AI systems (e.g., adversarial instances that contaminate the training of an AI-based cybersecurity tool).

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| **Enabling research topic** | **Description** |
| Definition of unwanted footprints | How should we formally define unwanted footprints in AI models? How should we incorporate application- or domain-specific requirements in the definition? |
| Footprint removal algorithms | How to design algorithms for removing unwanted footprints in AI models? What theoretical guarantees can such algorithms provide? How to benchmark the practical performance of such algorithms? How to handle complex learning paradigms (e.g., deep learning and reinforcement learning)? |
| Footprint removal auditing | How can we verify that a footprint removal request has been carried out by an organization? Alternatively, how can an organization provide formal proofs of footprint removal? |
| Evaluation of organizational trustworthiness | How can we monitor an organization’s digital footprint removal efforts over time to determine its overall compliance and trustworthiness? |

**AI for Science**

Scientific discoveries in the past decades have advanced our understanding of natural world, shedding light on everything from the evolution of stars, species of human ancestors, and discoveries of materials. Recently, there has been a growing interest in applying AI to accelerate scientific discoveries. For example, AI has been applied to automatically discover hidden state variables of physics phenomena. DeepMind’s AlphaFold has successfully predicted 3D structure of nearly all proteins known to science, accelerating innovation in drug discovery and biology. On one hand, AI has tremendous potential to impact science at the fundamental levels and revolutionize current practices. On the other hand, the gaps and open questions for AI fundamentals to apply to scientific discoveries remain unclear. AI for science remains largely unexplored.

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| **Enabling research topic** | **Description** |
| AI for natural law extraction and understanding | How can AI extract relevant latent features from high-dimensional data (e.g., videos, microscopy)? Examples: Method extracts state variables directly from video representations via a neural network with bottleneck latent embeddings; geometric manifold method to estimate intrinsic dimensionality.  How can AI extract physical laws from observations? Examples: Accelerated symbolic regression by exploiting graph modularity and symmetries in expressions; Monte Carlo sampling on manifold to identify dimensionality and conservation laws.  How to design AI models that are interpretable and can lead to insights? Examples: Use of gradient saliency to interpret found relationships through supervised learning models; SMILES representation with machine learning regression; automated anomaly detection and insights from experiments |
| Foundational AI models for fast, accurate, large-scale scientific discovery | How to train effective data-driven simulators for physical problems? Examples: Design new architecture to embed known inductive biases, recycling to improve prediction, and learning unlabelled sequences using self-distillation.  How to reduce simulators’ computational cost? Examples: New architecture to incorporate multiple scales; integration of supervised ML-derived variables into numerical solver for correction and interpolation.  How to maintain long-time stability and generalizability for dynamical systems? Examples: Physics-based constraints for neural networks, neural operators to improve generalizability even with less data. |
| AI for inverse design in science | How to automate the design of molecules/materials based on specific desirable properties (e.g., chemical)? Examples: Generation of molecular graphs using deep generative modelling that maintains chemical validity; AI models that are trained to generate molecules by learning the probability of the generation process of a large set of chemical structures; derivative-free/zeroth order optimization.  How to design derivative-free/zeroth order optimization strategies for inverse design? Examples: Incorporating expert knowledge into the derivative-free/zeroth order optimization strategies, optimizing potential energy surfaces of chemical systems, discovering design patterns via data-mining techniques.  How to effectively explore large high-dimensional space for inverse design? Examples: Generative models for out-of-distribution molecules/materials/experiment exploration, optimization that achieves novel solutions with diverse characteristics. |
| AI that maximizes a priori knowledge | How to design AI models that can be informed of physics by observational biases (e.g., sampling), learning biases (e.g., Lagrangian constrained loss function, transfer learning), or inductive biases (e.g., conjoint networks)? Examples: Utilizing analogies/knowledge from few and many body systems in quantum physics, Hamiltonian systems in classical physics; Explaining NN with optimization/physics-derived insights.  How to optimize and train AI models effectively given complex relationships and/or hard constraints that severely impact optimization? Example: non-L2 norms in pathology. |
| AI for data-sparse science | How can knowledge be maximized under resource constraints? Examples: Transfer learning methods; continual learning; new optimization algorithms for efficient sampling, especially with vast, discrete input spaces; representation learning in a small data regime. |
| Learning representations for scientific creativity | How to effectively explore large high-dimensional space for novel discoveries/experimental setups? Example: Creative adversarial networks to generate novel combinations, constraining generative models to produce out-of-distribution yet meaningful solution prototypes, exploration of creative compositions of primitive building blocks. |
| AI for quantum science | How can AI assist with high-dimensional optimization challenges? Examples: AI methods for quantum theory: searching of optimal parameters for quantum algorithms over infinite dimensional Hilbert space and quasi-probability functions with exponential scaling complexity; AI methods for quantum experiment: mapping desired states/operations onto quantum hardware given noisy logic gates and one to infinitely many functions; AI as the next generation of feedback control for complex systems. |

1. Singapore-based Institutes of Higher Learning and/or Research Institutions selected to host AI Singapore Research Programme projects will be eligible for indirect research cost (IRC) funding of up to 30% of the direct cost approved under the AI Singapore Research Programme. [↑](#footnote-ref-1)
2. The Google Scholar or DBLP identifier is an alphanumeric code to uniquely identify scientific and other academic authors and contributors. (refer to <https://dblp.uni-trier.de/>) [↑](#footnote-ref-2)
3. Represent % effort spent by the researcher in the project relative to his/her other team members. **The total must add up to 100%.**  [↑](#footnote-ref-3)
4. Represent % effort spent by the researcher in the project relative to his/her other job scope. Note that the PI is expected to commit **at least 20%** of his/her time and the Co-PI **at least 10%** of his/her time to this project. [↑](#footnote-ref-4)
5. *Institutes of Higher Learning (IHLs)*: National University of Singapore (NUS), Nanyang Technological University (NTU), Singapore Management University (SMU), Singapore University of Technology and Design (SUTD), Singapore Institute of Technology (SIT), Singapore University of Social Sciences (SUSS). [↑](#footnote-ref-5)
6. *Research Institutions (RIs):* A\*STAR Research Institutes/Centres/Consortia; CREATE Research Entities. [↑](#footnote-ref-6)