

Opening Remarks by Permanent Secretary for National Research and Development, Professor Tan Chorh Chuan at the AI for Science Nobel Turing Challenge Initiative Conference, 23 July 2024

Distinguished colleagues and friends, a very warm welcome to this AI for science conference. I want to thank our overseas speakers and participants who have travelled long distances to be here with us. Thank you very much indeed, we greatly value that.

I would like to start by thanking a number of people, firstly, Associate Professor Kedar Hippalgaonkar, and Professor Zhang Yang, from NTU, and NUS respectively, for co-organizing this meeting. It's organized jointly with the Nobel Turing Challenge Initiative led by Dr Hiroaki Kitano, CEO of Sony AI, Dr Jun Seita from RIKEN, and Professor Ross King from Chalmers University of Technology and Cambridge University. It is a great honour to host the Nobel Turing Challenge Initiative in Singapore for the first time. I also want to express our deep appreciation to Mr Ryo Haruta, Deputy Director, Basic Research Promotion Division, MEXT, for supporting this conference. I extend my warm welcome. It is a great pleasure for me to just make some opening remarks to try to set a broader context for the discussions that will occur today.

Singapore's National AI R&D Plan

National AI R&D Plan

Research capability platforms		Key enablers	
#1: Build peaks of basic AI research excellence in key areas	#3: Apply AI to drive major use cases to advance priority sectors	#6: Secure ample compute capacity	#8: Review RIE policies to facilitate implementation of AI initiatives
#2: Recruit, nurture and retain top AI talent	#4: Use AI to accelerate and boost research & new discoveries <small>AI for Science</small>	#7: Strengthen international linkages	
	#5: Ensure availability of high quality, context aware datasets		

In support of the
NAIS 2.0
NATIONAL AI STRATEGY

Late last year, Singapore developed its second version of its national AI strategy (NAIS2.0). Part of the national AI strategy has a substantial R&D component which we refer to as the national AI R&D plan. The R&D plan covers eight areas, starting with the talent, and a

number of other areas such as data, compute, international linkages, as well as the policies or regulations or guidelines for research. We are looking actively at them to try to ensure that they are facilitatory of AI initiatives given the speed at which AI research is developing in

Singapore and around the world. The central core of the R&D plan besides talent, are the three areas boxed in red in the slide:

- a. The first is there will be a strong focus to build peaks of basic AI research excellence in some key areas.
- b. The second is to apply AI to drive major use cases. And in our particular situation, we want to use these use cases to try to have a greater transformative effect on selected sectors.
- c. The third, which is the substance of today's discussion, is to use AI to accelerate and boost the research process itself.

AI for Science

AI for Science (AI4S)

What is AI for Science?

Use of AI to accelerate scientific inquiry and discovery, by automating and expanding the scale of hypothesis generation, experiments, and data analysis.

Why AI for Science?

Much greater speed and efficiency
a much greater part of research could be done computationally, and maximizing the yield of downstream wet-science experimentation.

Enables discoveries that might not otherwise be possible
e.g. AI can mine vast amounts of data to uncover patterns beyond human capabilities

4 When we speak about AI for science, we mean the use of AI to boost the research process itself, to accelerate the pace of scientific inquiry and to improve outputs of discovery. This can be done in a number of ways. I am speaking to a room full of experts, people who are

at the fronts of your field. You are all aware of how AI can deliver different ways of automating and in expanding the skill of hypothesis generation, and new ways of carrying out experimental research and data analysis.

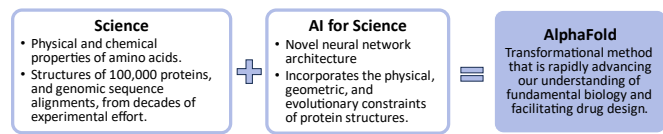
5 The reason why we and many others around the world are interested in AI for science or AI for research is the promise of being able to pursue research with much greater speed and effectiveness. A greater part of research, which would otherwise have to be done empirically could now be done computationally. There is the possibility that we can make best use of computational data to increase the likely yield of the wet bench experimentation. There is also the promise that AI could enable discoveries that might otherwise not be possible, for example, by mining vast amounts of data that human capabilities are incapable of doing.

AlphaFold

Accurate prediction of protein structures using AI



Before	AI	After
<ul style="list-style-type: none"> Predicting a single protein folding structure took <u>months to years</u>. Only 17% of human proteins have been experimentally determined in past 50 years. 		<ul style="list-style-type: none"> AlphaFold (2021) computationally predicted structures of 98% of human proteome in 930 GPU days; <u>minutes to hours</u> to predict a single structure. Accuracy validated against experimentally derived structures. AlphaFold 3.0 (2024) presents a significant advance, now enabling joint structure prediction of complexes including proteins, nucleic acids, small molecules.



4 computationally done within minutes to hours with a sufficiently high degree of accuracy. Without a doubt, AI has really caught on around the world.

6 Well, as I said, this is a roomful of experts. You are all aware of how AlphaFold was able to transform a process that was slow and laborious. Before, predicting single protein folding structures typically would take months to years, but with AlphaFold it can be

Global Initiatives in AI for Science

Surge in global initiatives in AI for Science:

Forbes
NSF Announces \$140 Million Investment In Seven Artificial Intelligence Research Institutes 4 May 2023

In 2023, NSF announced \$140 million for seven new AI research institutes, dedicated to areas including climate science and oceanography, education, materials and chemical synthesis, bioinformatics for next generation food systems, and agricultural resilience.

Japan to develop generative AI to speed scientific discovery
 Washington Post will be used for medicine and material development July 30, 2023

In 2023, the Japanese Ministry of Education announced \$2.2 billion in funding to support development of generative AI, that will derive insights from research papers and experimental images to generate hypotheses and expedite scientific discoveries, starting with a focus on medicine and materials exploration.

UKRI announces £80m investment into new UK research hubs for AI research 12 Feb 2024

In 2023-24, UKRI and EPSRC invested £80 million to fund nine new AI research hubs, six will explore AI for science, engineering and real-world data, to accelerate future AI innovations and advance applications in sectors such as healthcare, energy, smart cities and the environment.

U of T receives \$200-million grant to support Acceleration Consortium's 'self-driving labs' research April 26, 2023

In 2023, Canada First Research Excellence Fund (CFREF) awarded a \$200 million grant to University of Toronto's Acceleration Consortium, to support self-driving labs that combine AI, robotics, advanced computing to accelerate the discovery new materials and molecules.

self-driving labs in acceleration consortium.

7 We see a surge in global initiatives in AI for science, I've captured some recent initiatives in this slide from the the US, Japan and UKRI. We were recently at the University of Toronto congratulating them for receiving a CAD\$200 million dollar grant, the largest one in Canadian funding history to develop

NRF's AI for Science Scoping Report

In Singapore, extensive AI4S engagement with Research Community

- AI4S Scoping Report (<https://ai4science.sg>)
- Thematic workshops for domain deep dives (Apr-Jun) → Whitepapers outlining (i) problem statements (ii) bottlenecks (iii) methodology (iv) transformative opportunity / target outcomes

Domain	Leads: Domain expert, AI expert, bilingual expert	Date
Robotics Foundation Models	David Hsu, Lee Wee Sun, Choi Dongkyu	11 Mar
Complexity Science and Physics	Duane Loh, Lock Yue Chew	5 Apr
Earth and Climate Sciences	Dale Barker, Sang-Ho Yun	12 Apr
Genomics	Joanne Ngeow, Mile Sikic	12 Apr
Biomedical Sciences	Sebastian Maurer-Stroh, Mile Sikic	18 Apr
Financial Services	Bo An, Huang Ke-Wei	24 Apr
Chemical and Biological Manufacturing	Saif Khan, Wu Zhe	24 Apr
RNA Biology	Ashok Venkitaraman, Jinmiao Chen	25 Apr
Science, Software and Security	David Lo, Reza Shokri	2 May
Semiconductor manufacturing	J Senthilnath, Li Xiaoli, Aaron Thean	6 May
Materials Science and Chemistry	Kedar Hippaijanekar, Kostya Novoselov	8 May
Education	Tan Seng Chee, Ben Leong	9 May
Digital Phenotyping and Interventions	Robert Morris, Jimmy Lee	16 May
Hybrid Quantum Computing	Dario Poletti, Jose Ignacio Latorre	16 May
Sustainability	Madhavi Srinivasan, Yeoh Lean Weng, Arvind Easwaran	21 May
Healthcare and imaging	Rosa Qi Yue So, Daniel Ting, Ngiam Kee Yuan, Tan Cher Heng, Rick Goh	28 May
AI methods for Science (across domains)	B Low, YS Ong, Ng SeeKiong, Li Qianxiao, + Domain Experts	7 Jun

6 see the breadth of topics that were covered, as well as the types of people that were leading it in the slide.

8 In Singapore, we started looking at this at the end of last year, and through the hard work of my colleague at NRF, Professor Subodh and his team, he quickly put together a scoping report in the early part of this year, and then 15 thematic workshops were carried out. You can

9 The people in blue are domain experts. The people in red are AI experts, and the ones in green span both AI and domain. We were well supported. About 100 researchers in teams turned up and in just a few months, more than 1000 researchers in Singapore, including international collaborators, have come together to explore what we could do in this area.

Key takeaways from overseas study trips on AI

10 The National Research Foundation in Singapore undertook a series of overseas study trips as well. Let me distil our key takeaways from these trips.

Key takeaways for AI4S

Overseas Study Trips/Interviews (US, Europe, Japan and China)

- Bilingual domain-AI scientists will lead adoption of AI for research & Automated Labs
- Find synergies by generalising AI models, methods, and approaches to a class of problems
- Data to be driven by domain-specific use cases; Simulations & synthetic data to train model
- Compute requirements can vary significantly
- Pursue collaborations with industry

Insights from local Scoping Study / AI4S Workshops

- Singapore already has considerable ongoing AI4S effort in healthcare, advanced materials, life sciences, which this initiative can leverage.
- AI4S: national platform to enable deep collaborations between AI experts and domain researchers

11 The first is that *bilingual* scientists who can straddle between domain expertise in AI will be very critical in leading the development of AI for research. This offers incredible and exciting opportunities for younger researchers, of course, I leave the definition of younger, deliberately vague.

12 The second important takeaway that we gained was that there was a lot of scope for finding synergies by bringing different groups of people working on different types of problems together. For example, models or solutions, which were developed for a particular class of problems in a sector or scientific area could be generalised to attack the same type of computational problem in a completely different scientific domain. This abstraction and generalisation approach is something that we are very keen to try to encourage within Singapore. It could be a very powerful way of facilitating transfer learning that would allow us to speed up the application across many fields.

13 The third relates to data which we know is very critical. Cleaning up, procuring data and curating data, is very labour intensive. We saw across different sites the general approach was to curate data driven by specific domain use cases.

14 We also saw very impressive applications of simulations, modelling, and synthetic data to train models instead of using empirically derived data, this was particularly so in the case of robotics. There is scope to not just use empirically collected data, but modelling and simulation approaches could be useful to explore.

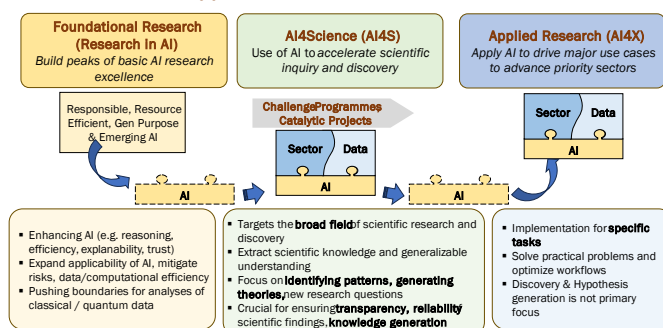
15 Compute requirements we know weigh a lot on researchers' minds. What we found was, depending on the type of AI research being pursued, a massive amount of compute requirements was not the norm all the time. In fact, several of our collaborators warned us that current algorithms are very inefficient, and therefore require excessive compute. We should develop much better algorithms and software that will allow us to use compute in a much more efficient way. This means training researchers who are not as familiar in high performance computing would be a very important step.

16 Finally, all of us recognise that industry holds a lot of expertise and pursuing deep collaborations with industry would be an important part too.

17 From our local scoping study, we were pleasantly surprised there were already considerable activity in AI for science across many areas, e.g., healthcare, advanced materials, life sciences. We can build upon this foundation of ongoing work. The AI for science initiative in Singapore could provide a very important platform that allows deep collaborations between AI experts and domain researchers across many different sectors.

AI for Science Initiative Platform– A Bidirectional flow of AI Methods & Approaches

Bidirectional flow of AI methods & approaches across Foundational Research, AI4S, & Applied Research

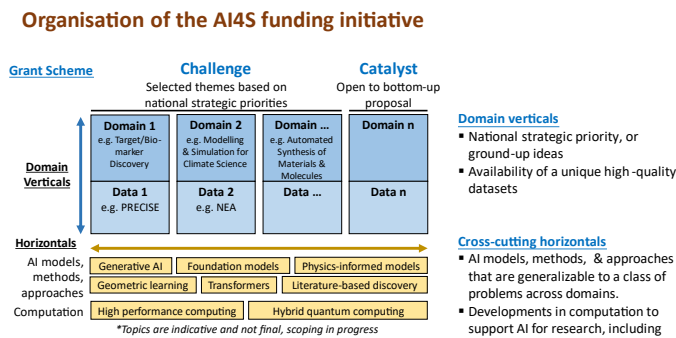


18 This slide, indeed a complicated one, expands on the idea I just shared. On the left there is foundational research and as I mentioned, we are seeking to build peaks of basic AI research excellence in Singapore, around responsible AI. This means

explainable AI, trustworthy AI, resource efficient AI, as well as general purpose and emerging AI techniques. Then, we create strong linkages and promote the use of models and algorithms developed from this process into the AI for science domain, which is illustrated in the middle of the slide. We do so by using AI to accelerate scientific inquiry and discovery. Some of the

approaches which are developed in both the foundational and AI for science areas could then flow through to the applied research area.

AI for Science Funding Initiative



19 This is broadly how we are organising the AI for science funding initiatives, which we will be putting up by the end of this year. There will be two main types of research proposals, a larger one in the region of about SGD \$10 million is a challenge research programme

based on defined thematic areas. The thematic areas will be designed in a way that is not prescriptive. We will define the broad themes, but we will leave a lot of space for ground up ideas to address these challenges. As shown in the slide, these challenges will be in different types of domains. We will assist with procurement of data for these different use case challenges.

20 On the chart's right, you can see we have smaller catalyst programmes, which are open for ground up proposals. It involves domains and data and the application of AI but will be open to ideas from any area at any field. Of course, there will be the horizontal areas comprising AI models, methods, approaches, and computation which will be part of this challenge. On the computation side, we are procuring additional compute resources to be able to support these programmes.

AI Revolutionising Science & Discovery

Summary

Revolutionizing scientific discovery with AI

- Pioneering new knowledge frontiers – deep learning, generative AI and foundation models
- Driving remarkable scientific discoveries
- Identifying ideas and trends in large complex datasets, predicting outcomes, simulating complex scenarios, and supporting literature management and data analysis

AI: Self-sustaining evolution ?

- Rapid approach towards inflection point
- Tremendous acceleration in AI progress – development of continuous and autonomous self-learning capability to achieve desired objective

21 In summary, we are in an exciting time where we see the promise that AI could contribute to revolutionising the scientific discovery process. It could lead to pioneering new knowledge in AI methods, and contribute to driving remarkable scientific discoveries. AI

will allow us to tackle large scale, complex data sets and problems that hereinto has been

difficult for us to do. Whether this will lead to a different kind of self-sustaining evolution of AI remains to be seen, but I think the promise is there.

22 In Singapore, as in most parts of the world, we would like to be part of this exciting journey. We like to work with collaborators across Singapore and with our many partners around the world to help advance this field. With that, I thank you once again, for being here today. It means a lot for us and I wish you a very fruitful, productive and exciting conference today and that you will also find some time to enjoy some parts of Singapore.

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