Why Fundamental Science Still Matters in the Age of AI:

A View from Computational Science

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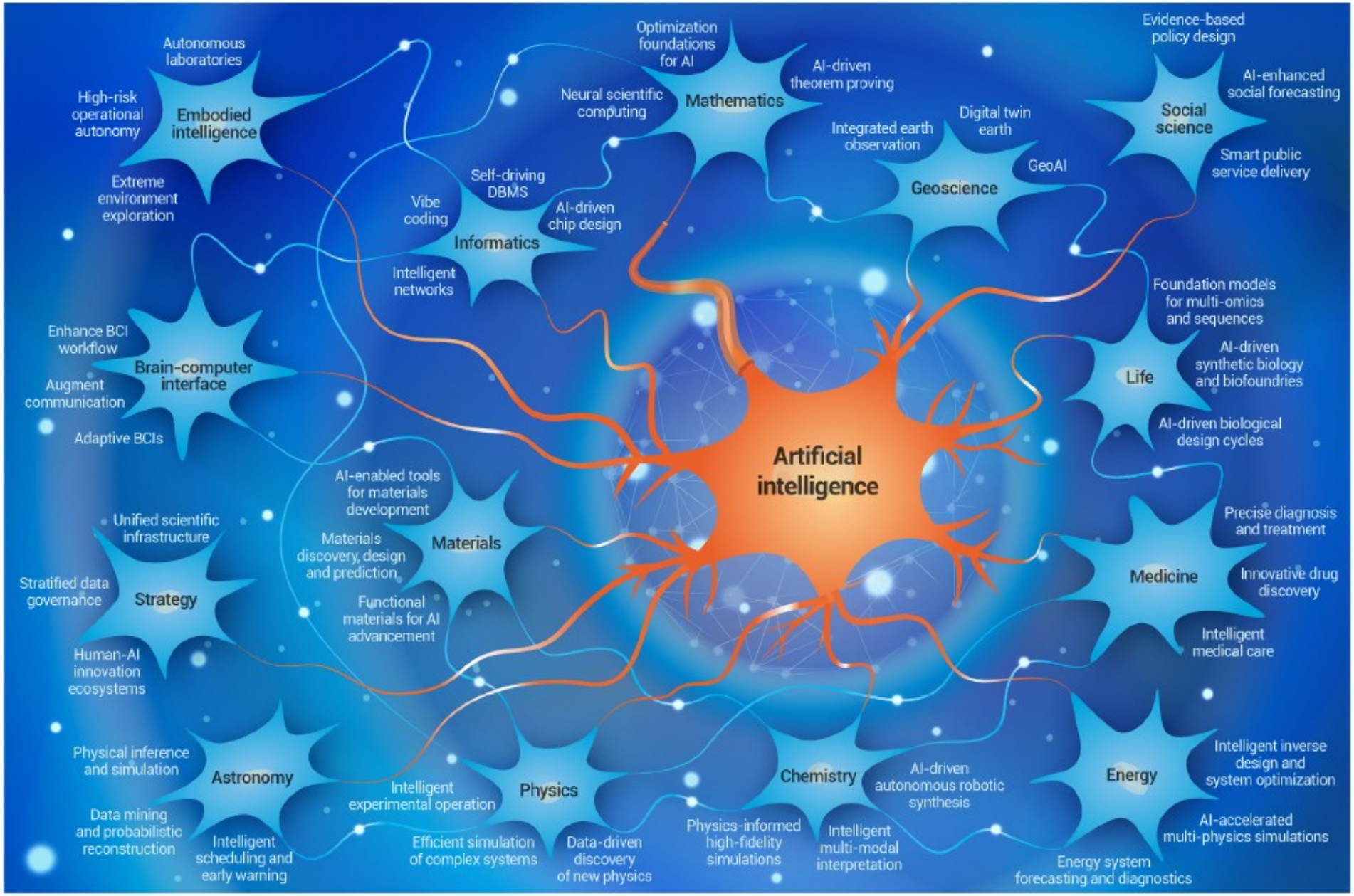
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Xu et al., *AI for science: Progress, challenges, and perspectives*, **The Innovation**, 2026, 7(11), 101530

Why it matters?

The Role of Fundamental Science:

Basic science provides **fundamental laws**, **principles**, and **mechanisms** governing physics, chemistry, biology, space, etc.

Without fundamental science, AI outputs are merely black-box predictions.

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1982

Hopfield network

Physics-inspired model of memory

2020

AlphaFold 2

Built on decades of structural biology and an open Protein Data Bank

2024

Two Nobel Prizes

Physics: Hopfield, Hinton.
Chemistry: Baker, Hassabis, Jumper

- **AI is built on fundamental science! Today's AI was yesterday's curiosity!**

The Role of Computational Science

| Computational science | Theory | Experiment |

- AI strengthens this role, but computational science provides the essential **bridge** among mathematical and physical principles, data, numerical methods, and scientific discovery.

- Many important scientific problems cannot be adequately addressed through **Theory** or **Experiments** alone

How Computational Science and AI Can Drive Research Excellence in Vietnam?

(1) AI impact on computational science

(2) Scientists should change the way they conduct research

(3) Vietnam needs to change to achieve research excellence

AI Impact on Computational Science

- AI *improves* Computational Science: Faster computation
  (Replacing thousands of expensive finite element simulations with a trained surrogate model for rapid prediction)
- AI *transforms* Computational Science: New ways of modelling/solving problems
- AI *enables* Scientific Discovery: New scientific understanding - identifying relationships and mechanisms that were previously unknown.

AI Impact on Computational Science

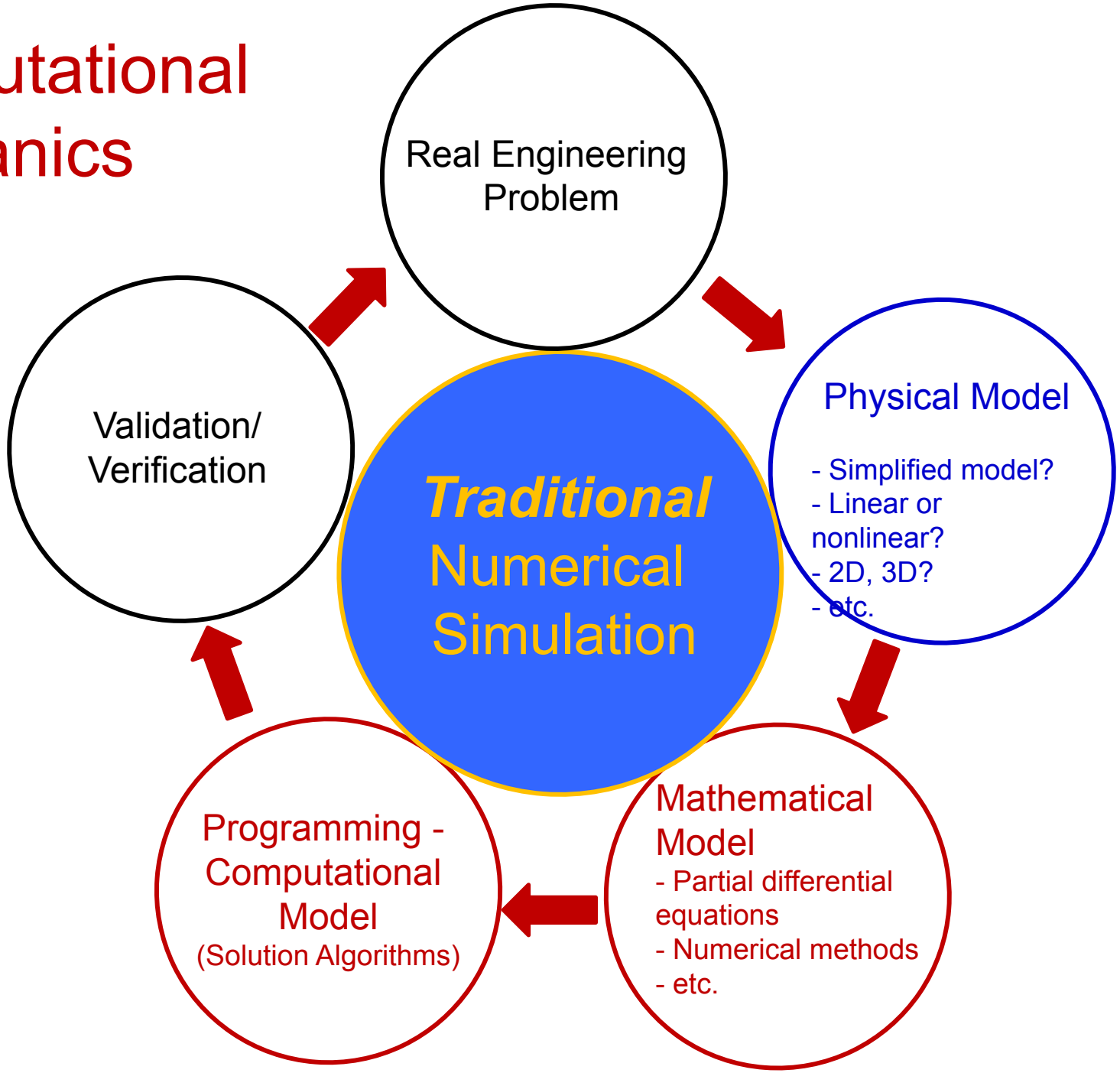
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AI does not automatically provide:

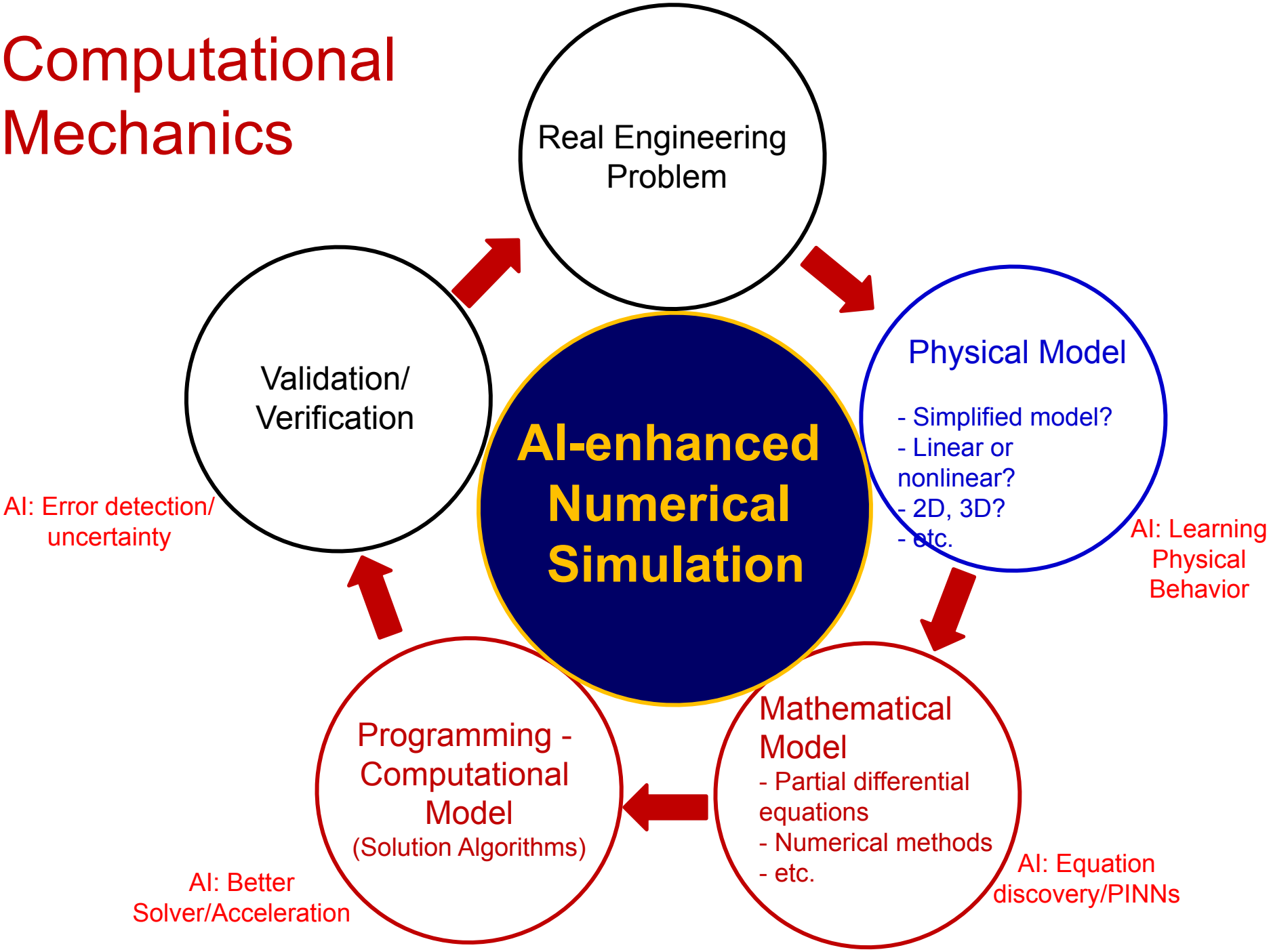
- Physical understanding of a phenomenon
- Correct governing equations
- Reliable predictions outside its training data
- Experimental validation of scientific hypotheses

The role of scientists remains essential: defining meaningful questions, establishing physical principles, evaluating scientific evidence and validating discoveries.

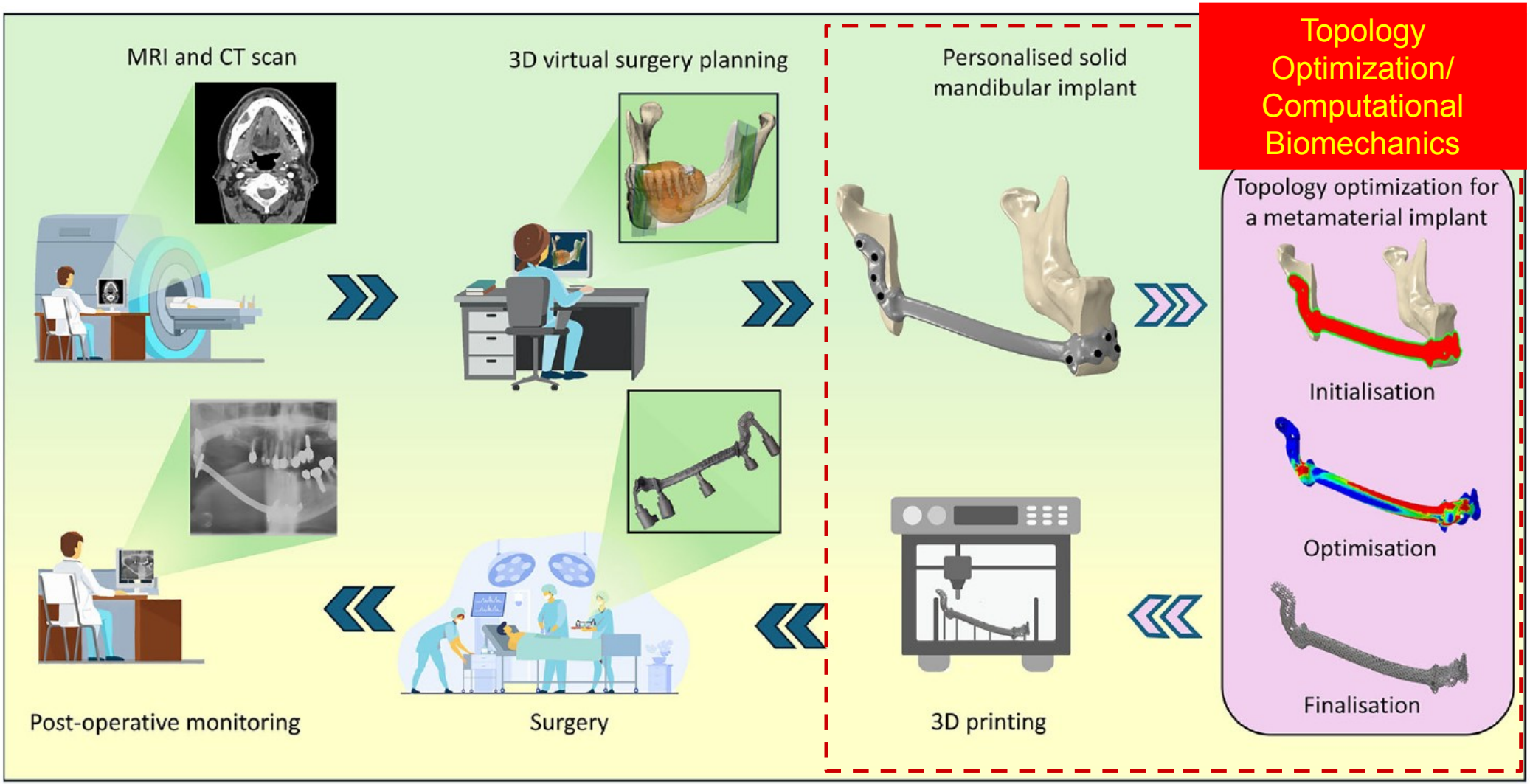
Computational Mechanics



Computational Mechanics



AI-driven Topology Optimization for a mandibular implant using Meta-materials



The New Challenge: Can We Trust AI?

Example: Consider a student using AI to solve a computational mechanics problem

AI provides	What the student may fail to recognize
• Governing equations	*Are the equations physically correct?*
• Mathematical derivation	*Are there hidden mathematical errors?*
• Numerical algorithm	*Is the method stable and convergent?*
• MATLAB/Python code	*Does the code implement the intended physics?*
• Numerical results	*Are the results physically meaningful?*
• Scientific explanation	*Is the interpretation scientifically justified?*

AI can generate solutions. But how to verify them?

Scientists must change their way to conduct their research

- The future scientist is not simply *a user* of AI.
- From solving known problems to *asking better questions*
- From limited information to *data-driven discovery*
- From conventional methods to *hybrid* scientific methods
- From individual research to *AI-assisted* collaboration
- From accepting results to *rigorous* scientific verification

Vietnam needs to change to achieve research excellence

It requires changes in **research culture and organization**:

1. Pursue original and ambitious fundamental questions
2. Build the capacity to formulate and solve important scientific problems, rather than simply adopt advanced technologies.
3. **Build strong research groups**
4. **Provide long-term research funding**
5. Strengthen international partnerships

Concluding Remarks:

- The future belongs not only to those who use AI, but to those who advance science with it.
- AI does not replace fundamental science. It makes fundamental science even more important, while opening new ways to conduct it.
- Fundamental science makes AI more powerful.

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For Vietnam, the opportunity is not simply to adopt AI, but to use it to build a stronger scientific foundation, empower outstanding researchers, and contribute new knowledge to the world.

Publish clear rules on how applicants may use AI to write proposals, and require disclosure.

THANK YOU!