AdaLab

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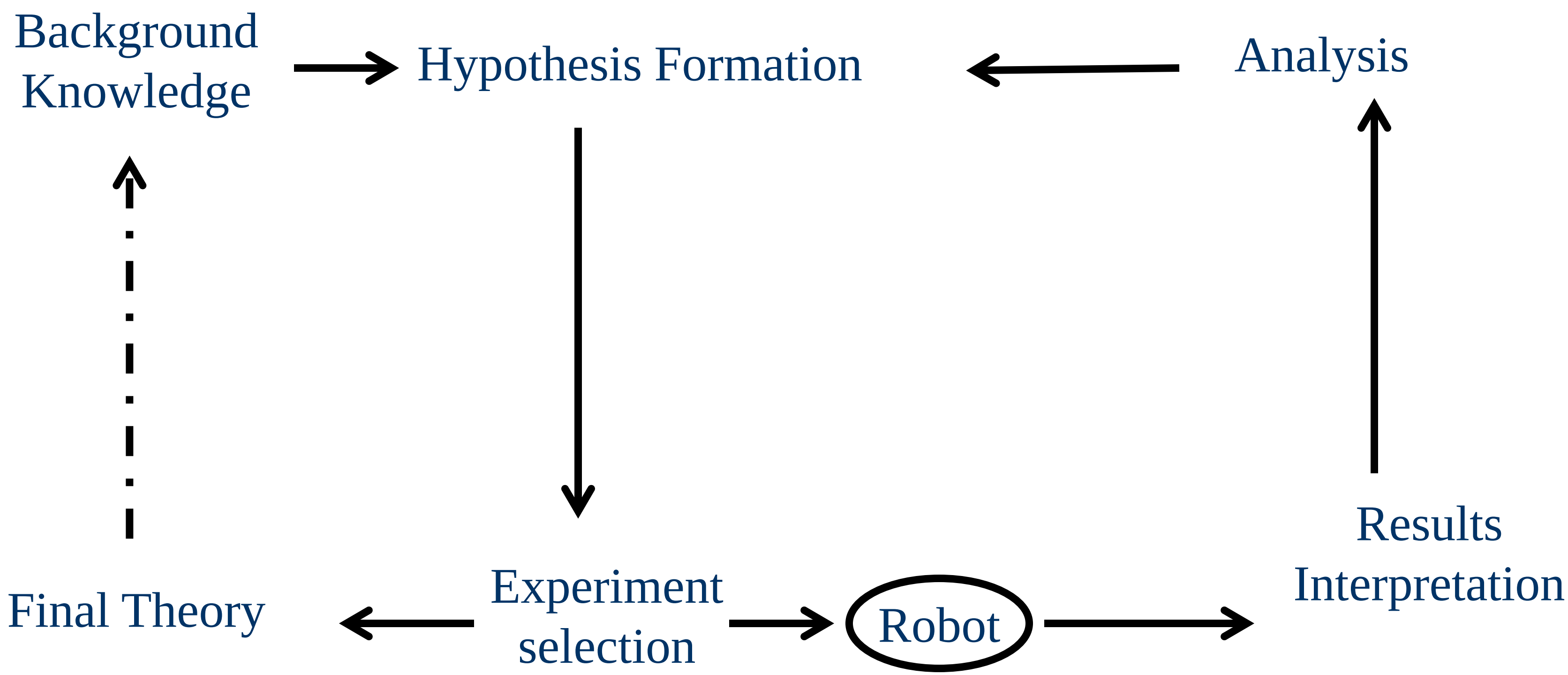
- Adaptive Automated Scientific Laboratory (AdaLab)
- Adaptive Machines in Complex Environments
- Start Date: 1.4.15

Scientific Background

The Concept of a Robot Scientist

Computer systems capable of originating their own experiments, physically executing them, interpreting the results, and then repeating the cycle.



Scientific Goals

- We aim to integrate the scientific method with 21st century automation technology.
- We aim to make scientific discovery more efficient: cheaper, faster, better.

- Our vision is that within 10 years many scientific discoveries will be made by teams of human and robot scientists.
- This collaborations will produce scientific knowledge more efficiently than either could alone.

Scientific Goals

- We propose to develop a framework for semi-automated and automated knowledge discovery by teams of human and robot scientists.

- This framework will integrate and advance: knowledge representation, ontology engineering, semantic technologies, machine learning, bioinformatics, and automated experimentation.

- We will evaluate the AdaLab framework on an important real-world application in cell biology with biomedical relevance to cancer and ageing.

The Diauxic Shift

- Yeast (*S. cerevisiae*).
- First turn sugar into ethanol.
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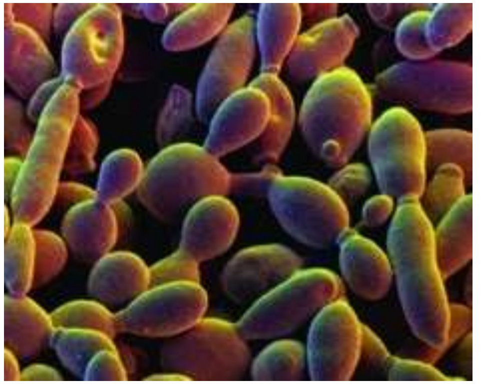
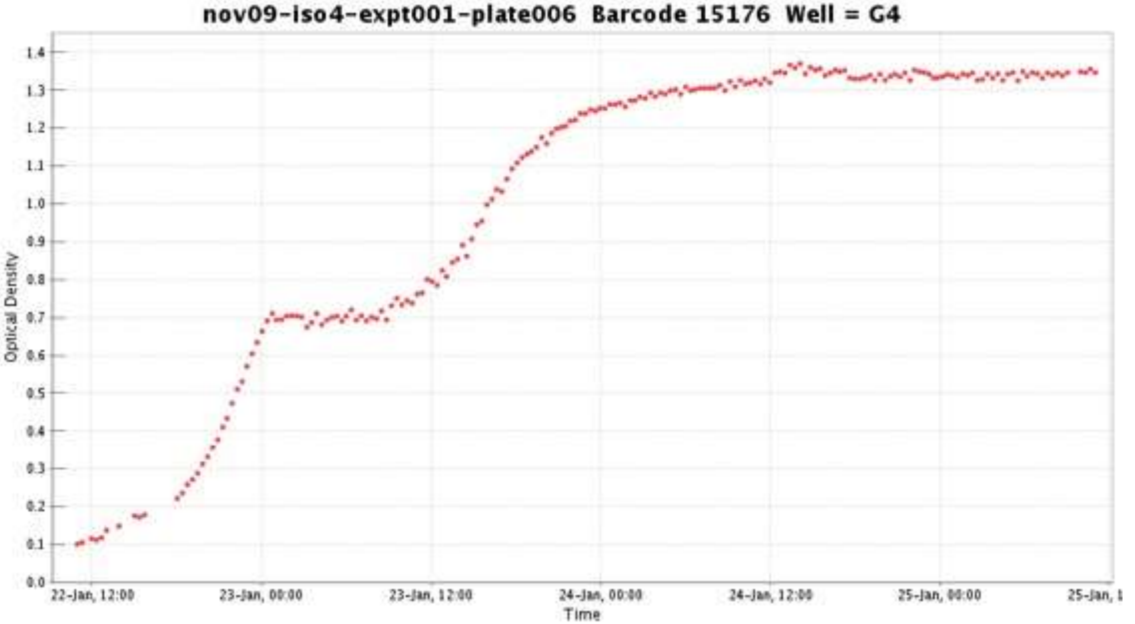


- Cancer
- Ageing



Eve

- Eve running

Partners

Brunel University: Coordinator

- In London, near Heathrow airport.
- Over 15,000 students and 1,000 academic staff from 113 different countries
- Coordinates 11 FP7 EU projects, and a partner in >50 other EU projects
- Secured >€18 M in European funding for the last two years
- A wide range of scientific expertise, from robotic engineering to the Centre of Systems and Synthetic Biology

Role in Project: Knowledge representation

- The formal machine processable representations of the principle data and knowledge entities involved to the project, e.g. equipment, processes, participants, hypotheses, data, results.
- A declarative language for ML and probabilistic reasoning components.
- A knowledge base about the yeast diauxic shift.
- A communication mechanism between robot and human scientists.

University of Manchester

Ross D. King, Professor of Machine Intelligence,
ross.king@manchester.ac.uk

- Manchester
- North of England
- Alan M. Turing
- Manchester 'Baby'

- Role in Project
- Head of Research
- Robot Scientists: Eve.
- Biological application
- Machine Learning

Partner KULeuven (Belgium)

- PI: Jan Ramon
- Specificity:
  - Data mining in graphs
  - Active learning
  - Probabilistic models
- Related projects:
  - MiGraNT (theory for data mining in networks)
  - InSPECtor (Proteomics experimental research)

- Role in ChistERA AdaLab:
  - Modeling uncertain knowledge
  - Hypothesis generation
  - Optimisation of experiment selection
  - Probabilistic inference
  - Algorithms for network data

Laboratoire d'Informatique de Paris-Nord: LIPN

- Celine Rouveirol
- LIPN is asssociated with CNRS (UMR 7030). Research groups in *Combinatorics*, *Combinatorial Optimisation*, *Algorithmics*, *Logic*, *Software Engineering*, *Natural Language*, *Machine Learning*. The group involved in the project is: Machine Learning and applications.
- Research in this team focuses on three main topics:
  - Algebraic and logical models of learning,
  - Collaborative and transfer learning,
  - Learning structures from heterogeneous data.

Role in the Project

- Inductive Logic Programming: incremental theory revision, active learning, (deterministic) action model learning, learning from ambiguous relational examples.
- Complex systems analysis: community extraction, link prediction in multiplex networks
- In collaboration with UPMC-LIP6, collective learning (multi-agent), distributed abduction.
- In collaboration with Evry University, inference of regulation networks from gene expression datasets.

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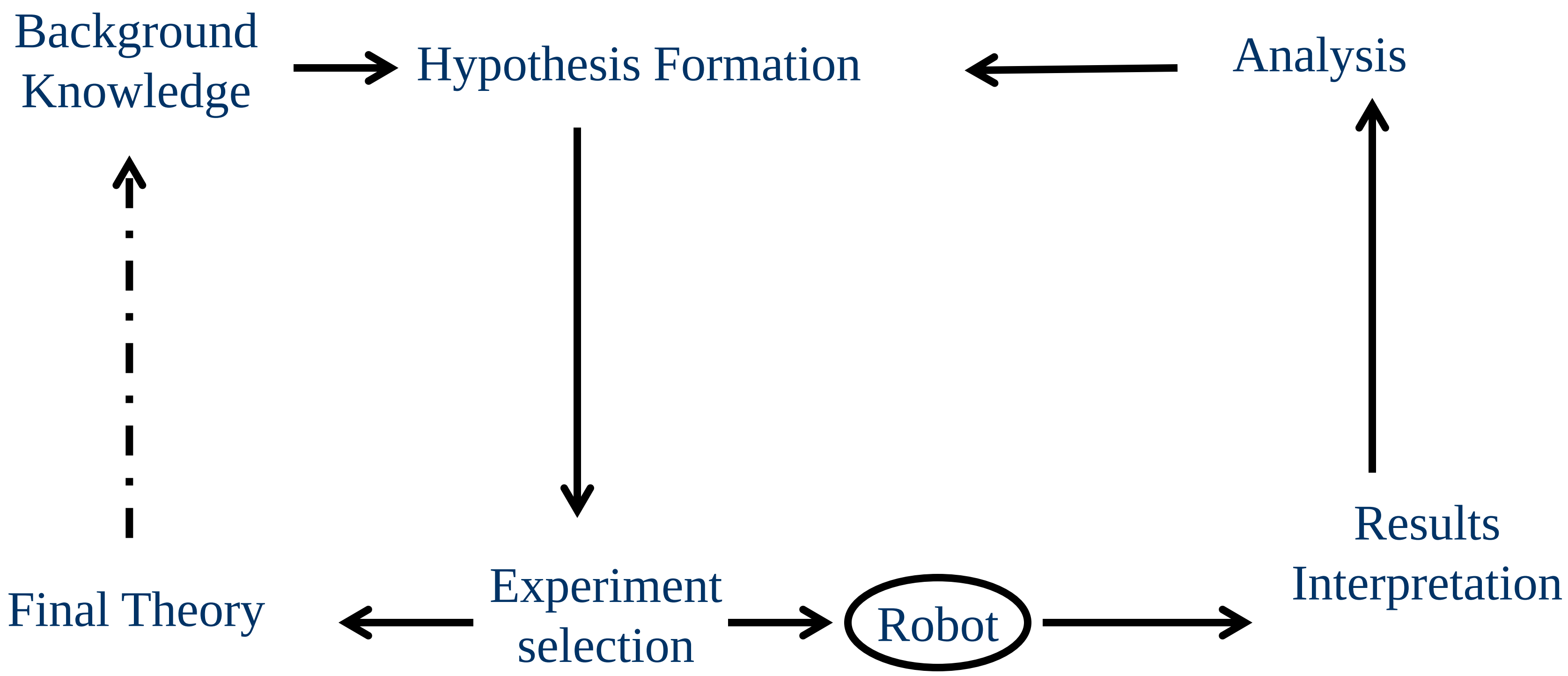

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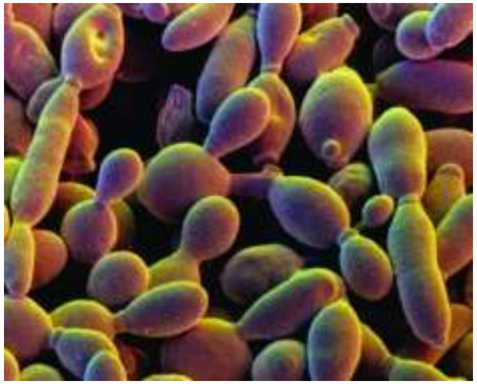

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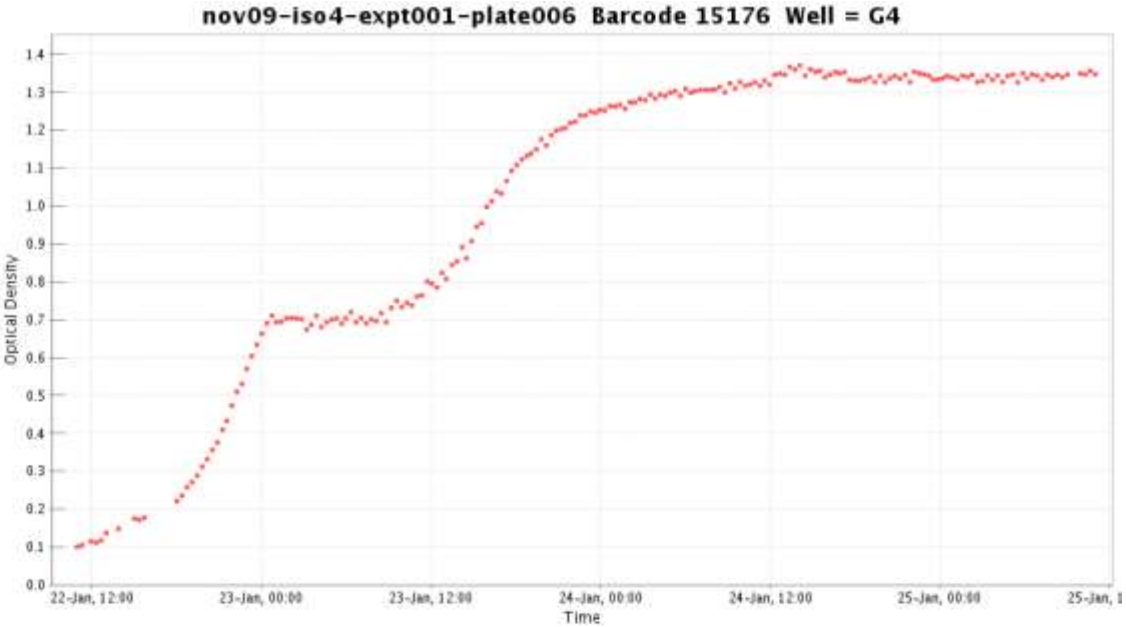

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Institute of Systems & Synthetic Biology (iSSB-UE)

Mohamed Elati

- The Institute of Systems and Synthetic Biology is a research unit of University of Evry and CNRS. The iSSB is located on the Genopole campus, the leading BioPark in France, near Paris.
- Research areas: machine learning, computational and systems biology, bioinformatics.
- AdaLab:
  - Reconstruction of context-specific molecular networks about yeast diauxic shift
  - Integration of molecular network data, to reconstruct active ontology and selecting experiments

Key challenges and potential impact of the project

Key Challenges 1

- The proposed AdaLab needs to be:
  - *autonomous and perceptive to human requirements* (its scientific collaborators).
  - *able to continuously learn, adapt and improve in the "real world" complex environment* of scientific research.
  - capable of continuous cycles of scientific hypothesis formation and experimentation that will improve its scientific knowledge (models).

Key Challenges 2

- *Integrating a systems approach*, with the research involving collaboration between experts in: robotics, machine *learning, logical and probabilistic inference*, *semantic technologies*, and yeast microbiology.

- *Integrating* high-level reasoning about scientific knowledge *with the control of low-level robotic movements* to execute experiments.

- Develop *a protocol for communication between human and robot* scientists.

Key Challenges 3

- Scientific knowledge is inherently uncertain. Therefore within the AdaLab framework we need to develop Bayesian methods that make *inferences* and plan experiments *under uncertainty*.
- Scientific knowledge is best represented using *logic*. To *integrate logic with probabilities* we will use statistical relational learning, and develop an ontology for *representing uncertain knowledge*.
- The success of the AdaLab framework will be objectively determined by quantitative measurements of the different system components, and the scientific knowledge generated.

Key Outputs

- An AdaLab demonstrated to be greater than 20% more efficient at discovering scientific knowledge (within a limited scientific domain) than human scientists alone.
- A novel ontology for modelling uncertain knowledge.
- An efficient communication mechanism between human and robot scientists.
- New machine learning methods for the generation and efficient testing of complex scientific.
- Novel biomedical knowledge about cell biology relevant to cancer and ageing.

Potential Impact

- Science is the greatest generator of economic wealth (through developments in technology).
- Science is the greatest driver of better health (through development in biomedical science).

- The AdaLab framework will contribute to *realising Europe's 2020 strategy for smart, sustainable and inclusive growth* chist-era

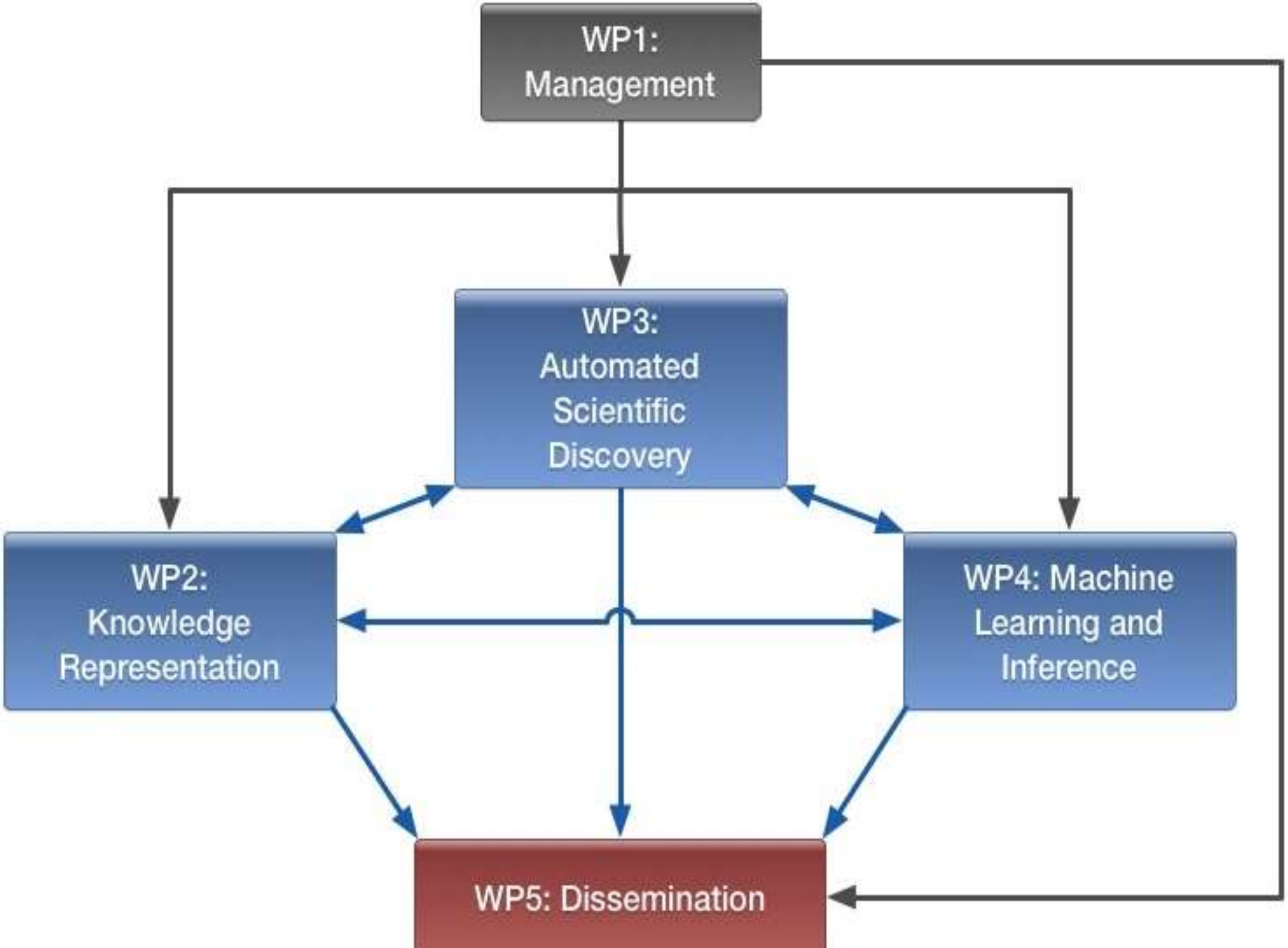
Potential Impact

- Intelligent laboratories have the potential to speed up the technological progress.
- Such an increase would lead to more scientific discoveries, better technological solutions, and new products.

- For example new better drugs could be delivered to the market faster and cheaper. Currently, ~25Billion € is spent annually within the EU on pharmaceutical research. Most of this is spent on late-stage trials (which are less amenable to automation), but we conservatively estimate that ~10% is amenable to the AdaLab framework.

Planning

Work packages



Work plan

- Five interlinked WPs.
- The proposed AdaLab framework will be developed in three cyclic iterations.
- The main software components will be incrementally released and updated.
- All projects outputs will be made available to the research community by the end of the project.

The End of the Beginning of AdaLab