Synthesis Panel
Summary by Timothy Gardner, CEO

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Advanced and Automated Workflows
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Digitization is driving a reshaping of how we do science

Science accelerated by: Calculators -> Computers -> Supercomputers -> AI -> Automation -> Closed Loop Automated Experimentation?

Why?

Make science better, faster, more capable, more scalable, more automated

Shared, structured, machine-computable data is critical to that

Well-structured workflows give such data and its verifiable provenance

Workflows - old idea but hard to adopt

People love writing them, don't like using

Scientist perceive low value

Barriers to adoption

“Intrinsic complexity means that participants are always working at 100% cognitive load. I don't think simplicity of UI is the solution. We need to understand our objectives.”

Crossing the chasm

from Early adopters …
to Fast followers …
to Early majority **<-- This is what we are striving for**

What's needed for successes at scale?

Examples: Synthetic chemistry, Higgs Boson, Digital Sky

Unsolved issues: better experiment design, better data science knowledge, better models for collaboration, importance of well-posed / well-scoped problems

Need for standards

But standards are evolutionary and hard to mandate

Terminology (at the language normalization level)

Workflow, process, specification, execution, data flow
Inputs, outputs, operations, etc.

Encapsulated objects

Biocompute
CommonWL
Riffyn

Human readable, machine computable, standardized, interchangeable, sharable

Pathway to standardization by practical adoption?

Need for infrastructure

Secure but open and sharable data handling (before privacy)

Science is a workflow/process

We know that intuitively (hypothesis, experiment, analysis, conclusion)

Workflow starts in the lab with the experiment, not just the computation

We don't always perform it that way, but we need to. We do this in all other fields of human endeavor