1. Motivation

2. Infrastructure

3. AiiDA graph, nodes, link types and their properties

4.QueryBuilder with full graph traversal

5. AiiDA plugin registry

6. Flexible and powerful workflow language and engine

7. 65x performance boost and 45x space improvements

8. Caching

9. Extended testing and continuous integration

10. Knowledge transfer

AiiDA - Automated interactive infrastructure and database for computational science

Remote management
Coupling to data
High-throughput
Automation
Data
Sharing
Environment
High-level workspace
Scientific workflows
Data analytics
Social ecosystem
Standardisation
Repository pipelines

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