

Center for Integrative Bioinformatics (CIBI Konstanz)

KNIME Analytics Platform for the Reproducible

Analysis of Life Science Data

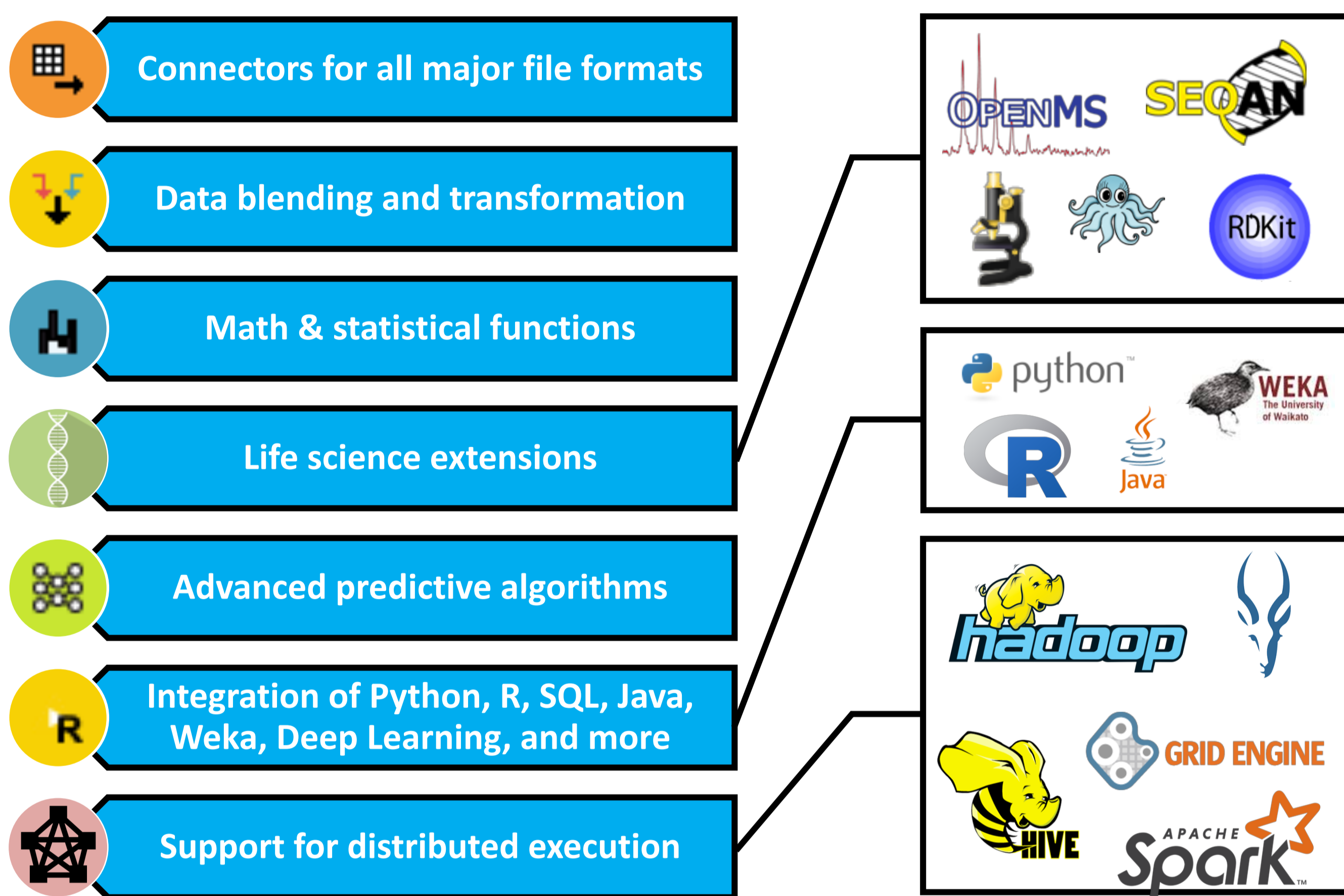
FKZ: 31A535C

Alexander Fillbrunn, Michael Berthold

Short description of the project

KNIME:

- Open source workflow platform
- More than 2000 workflow nodes for various data processing tasks
- Consulting, training, and support for users and developers
- Integration of CIBI partner tools and many others



de.NBI services

KNIME:

- Consulting and software support for both users and developers
- Training users and external developers
- Integration of external tools and repositories via workflow nodes
- Improvements to software documentation and teaching material
- Two software releases per year
- Maintenance of build and test infrastructure

de.NBI cloud activities

- KNIME in the de.NBI cloud
- Container based deployment on compute nodes
- Singularity for secure HPC
- File transfer via SFTP, Shared File System and direct transmission

Staff

- 1 FTE paid through de.NBI
- All positions are currently filled

Progress report

KNIME:

Distributed Execution in the cloud

- Cluster execution on many queuing systems
 - Torque
 - Sun/Open Grid Engine
 - SLURM
 - Moab
- Setup of distributed OpenMS workflow execution
 - With SLURM on the de.NBI Cloud
 - With Sun Grid Engine at the HZI in Braunschweig
- Consulting and software support

Containerization

- Improved workflow and software containerization with Singularity and Docker
- Easy deployment of instances in the cloud
 - Common settings and plugins
 - Common dependencies
 - Common Python and R runtimes
- Common Workflow Language support
 - Run KNIME workflows via CWL (Cooperation with IBISBA Project)

Training and education

- Revised training material
- Developer, user meetings, and conferences
- Online lectures and tutorials
- Blog posts and video lectures
- 2 articles in Linux Magazin, Germany, 1 article in Linux Pro Magazine, US

Community

- KNIME Workflow Hub (former Social Workflow Repository)
 - Website for showcasing example workflows
 - Community can download, comment and rate workflows

de.NBI training and education

4 training events in 2018

Mar 2018	(Berlin, DE):	Life Science workshop at the KNIME Spring Summit 2018
Jul 2018	(Konstanz, DE):	Data Science for Life Sciences course at the University of Konstanz
Sep 2018	(Konstanz, DE):	de.NBI CIBI KNIME Cluster and Cloud Hackathon
Sep 2018	(Berlin, DE):	KNIME course at the 2 nd CIBI User Meeting

Selected Publications

KNIME for reproducible cross-domain analysis of life science data
A. Fillbrunn, C. Dietz, J. Pfeuffer, R. Rahn, G. A. Landrum, M. R. Berthold; *Journal of Biotechnology*
Workflow-basierte Datenanalyse
A. Fillbrunn, M. Horn; *Linux Magazin* 04/2018
Maschinelles Lernen mit Knime in der Praxis
A. Fillbrunn, M. Horn; *Linux Magazin* 10/2018