



CloudBroker

High Performance Computing
Software as a Service

Integration in KNIME

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HPC Applications in KNIME

KNIME works great for constructing, executing and exchanging workflows:

- Focus is on high throughput computing and rich client experience

Current support for batch-oriented, number-crunching, high performance computing (HPC) applications:

- Application-specific nodes to connect to particular external HPC software
- KNIME Cluster Execution to run existing nodes on an SGE-based cluster
- Build your own interface to HPC software and resources using SSH, Java, Python, web service or similar nodes
- Implement your own solution

Problems with HPC Applications

You have to:

- Build, operate and update your own cluster infrastructure
- Buy long-term licenses and support external software
- Make sure that the needed KNIME nodes or implementations are available or developed

This means:

- Complex and time-consuming setup, maintenance and change procedures
- High initial costs for hardware and software
- Probably some own programming efforts
- Need for specialized personnel
- No flexibility for special projects, testing, varying load, etc.

Cloud Computing

Computer resources (infrastructure, platforms, software) provided as a service via the internet, on demand in a self-service manner

This means:

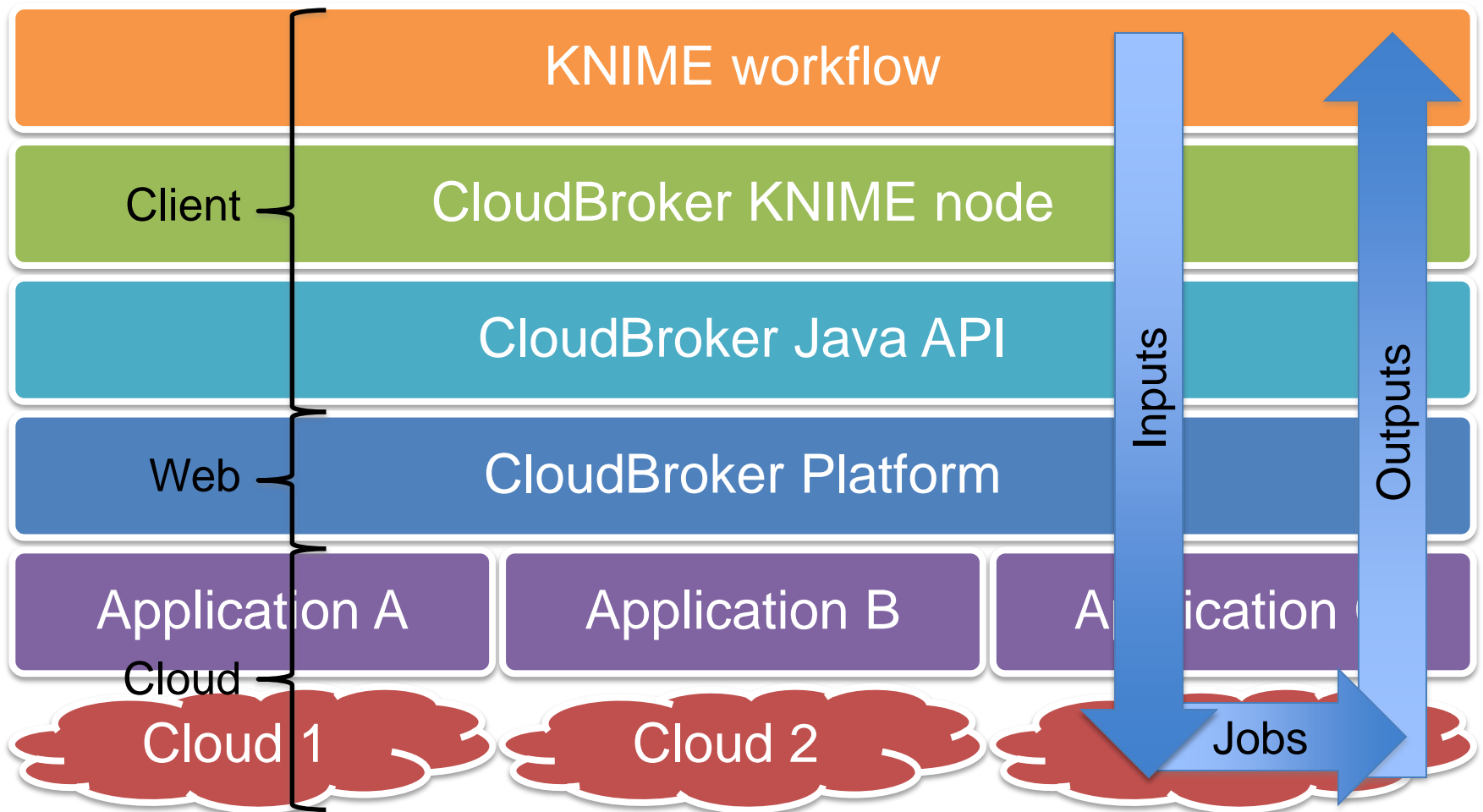
- Minimal initial investments in cost and time
- You only pay for what you actually use
- Nearly unlimited scalability

Your advantages:

- Increased flexibility
- Concentration on core competencies
- CapEx substituted by OpEx
- Over- or underutilization replaced by elastic scalability

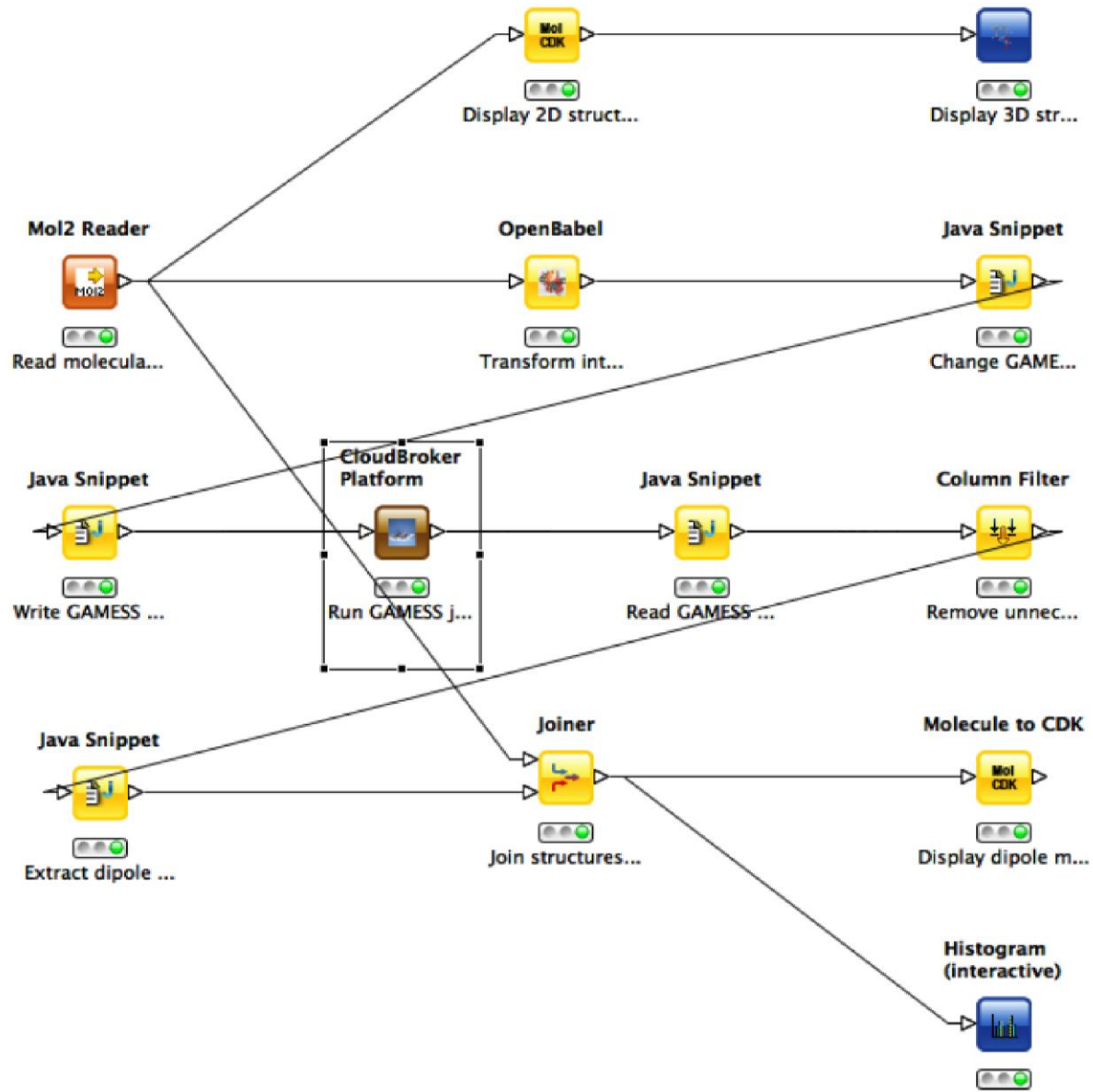
**CloudBroker
Platform =
Application
store for high
performance
computing in
the cloud**

Integration into KNIME



Example Workflow

- Goal: Compute the quantum chemical dipole moments for a number of molecules
- Application: GAMESS (General Atomic and Molecular Electronic Structure System, <http://www.msg.chem.iastate.edu/gamess>)
- Data set: Some ligands from DUD (Directory of Useful Decoys, <http://dud.docking.org>), provided by KNIME



Advantages



- Access to a number of different HPC applications from various domains (life sciences, chemistry, engineering, etc.)
- Easy integration into any type of KNIME workflow
- No need to buy, install or operate any HPC hardware or software
- Scalable cloud infrastructure
- Pay per use charging model
- Just registration in the CloudBroker Platform needed
- Deployment of your application into the platform also possible

Availability



- CloudBroker Platform preview version available to selected users
(<http://www.cloudbroker.com/index.php/platform>)
- Applications: GAMESS, BLAST, AutoDock, Gromacs, X! Tandem, OpenFOAM, Rosetta (upcoming)
- Clouds: Amazon Web Services, IBM Cloud (upcoming)
- CloudBroker KNIME node to be released together with next platform version (expected April 2011)
- Future plans: Possibility to execute whole KNIME workflows in the cloud via the platform



Thanks! – Questions?

Thanks to the CloudBroker Team and to KNIME!

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