

WebからKNIMEをつかう話

2019.09.21@沼津

おまけ : KNIME

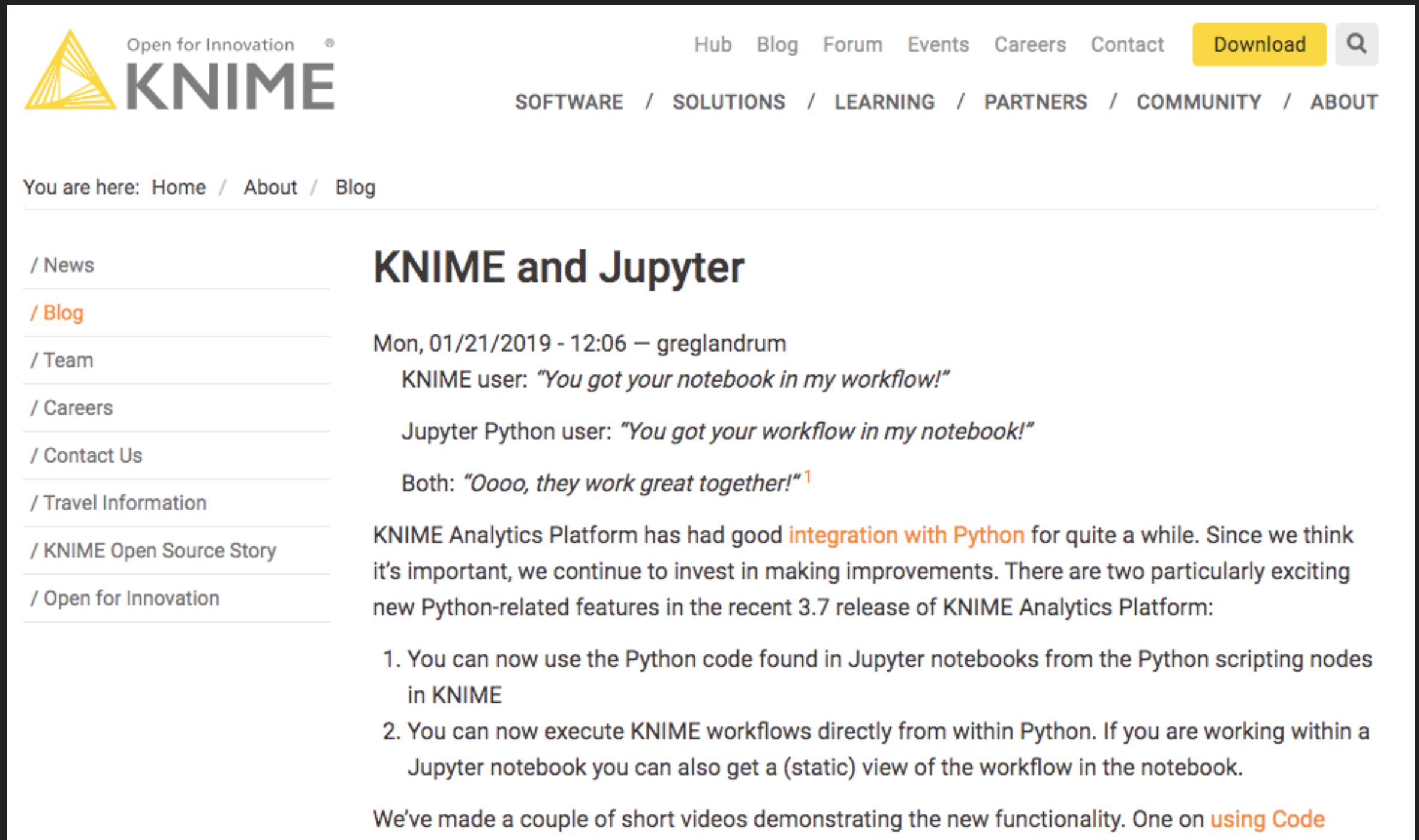
@kochi0603

今日の話でちょっと出てきた。


- ▶ KNIMEを自動化
 - ▶ Batch_modeでできるよ
 - ▶ KNIME_batch_mode_20190921_kochi.pdf に書いた
- ▶ KNIMEをWebで
 - ▶ Batch_modeでもできるけど、KNIME.pyの方が良さげ


- ▶ 1月ごろ、@dr_greg_landrum、@iwatobipenがJupyter-KNIMEの連携の紹介をしてた
 - ▶ KNIME.py の作りが良さそう。
- ▶ WebからKNIMEをBatchモードで起動するのは、
 - ▶ 起動までちょっと待つ
 - ▶ KNIMEを起動しっぱなしに出来ないのでは
 - ▶ Webサービスにはしにくい
- ▶ Flaskで、KNIME.py経由でKNIMEを実行させる

<https://www.knime.com/blog/knime-and-jupyter>



The screenshot shows the KNIME website's blog page. The header includes the KNIME logo with the tagline 'Open for Innovation', navigation links for Hub, Blog, Forum, Events, Careers, and Contact, a yellow 'Download' button, and a search icon. A secondary navigation bar lists categories: SOFTWARE, SOLUTIONS, LEARNING, PARTNERS, COMMUNITY, and ABOUT. A breadcrumb trail indicates the current location: Home / About / Blog. A left sidebar contains links to News, Blog (highlighted in orange), Team, Careers, Contact Us, Travel Information, KNIME Open Source Story, and Open for Innovation. The main content area features the article title 'KNIME and Jupyter' in large bold letters. Below the title is the date and author: 'Mon, 01/21/2019 - 12:06 — greglandrum'. The article text includes two quotes: 'KNIME user: "You got your notebook in my workflow!"' and 'Jupyter Python user: "You got your workflow in my notebook!"', followed by a combined quote: 'Both: "Oooo, they work great together!"¹'. The main text paragraph states that KNIME Analytics Platform has had good integration with Python for quite a while and continues to invest in improvements, mentioning two new Python-related features in the recent 3.7 release. These features are listed in a numbered list: 1. You can now use the Python code found in Jupyter notebooks from the Python scripting nodes in KNIME; 2. You can now execute KNIME workflows directly from within Python. If you are working within a Jupyter notebook you can also get a (static) view of the workflow in the notebook. The paragraph concludes with a mention of short videos demonstrating the new functionality, with a link to 'using Code'.

Open for Innovation  **KNIME**

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KNIME and Jupyter

Mon, 01/21/2019 - 12:06 — greglandrum

KNIME user: *"You got your notebook in my workflow!"*

Jupyter Python user: *"You got your workflow in my notebook!"*

Both: *"Oooo, they work great together!"¹*

KNIME Analytics Platform has had good **integration with Python** for quite a while. Since we think it's important, we continue to invest in making improvements. There are two particularly exciting new Python-related features in the recent 3.7 release of KNIME Analytics Platform:

1. You can now use the Python code found in Jupyter notebooks from the Python scripting nodes in KNIME
2. You can now execute KNIME workflows directly from within Python. If you are working within a Jupyter notebook you can also get a (static) view of the workflow in the notebook.

We've made a couple of short videos demonstrating the new functionality. One on **using Code**

<https://iwatobipen.wordpress.com/tag/knime/>

Call Knime from Jupyter notebook! #Chemoinformatics #RDKit #Knime

🕒 23/01/2019 📁 diary 🏷 chemoinformatics, knime, RDKit

I read exiting blog post yesterday! URL is below.

<https://www.knime.com/knime-blog-general>


@dr_greg_landrum developed very cool tools which can call knime from jupyter notebook and can execute jupyter notebook from knime.

Details of the tool is described in the [Knime blog post](#). I am interested the tool and I can't wait to try it in myself. So I used it from my mac book pro. At first I installed python knime package via pypi.

▶ 実際に使うには、

2019.02.09

<https://pypi.org/project/knime/>




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knime 0.9.5

✓

[Latest version](#)


`pip install knime`





Last released: Dec 24, 2018

Tools for reading and executing KNIME workflows.

Navigation

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 [Release history](#)

 [Download files](#)

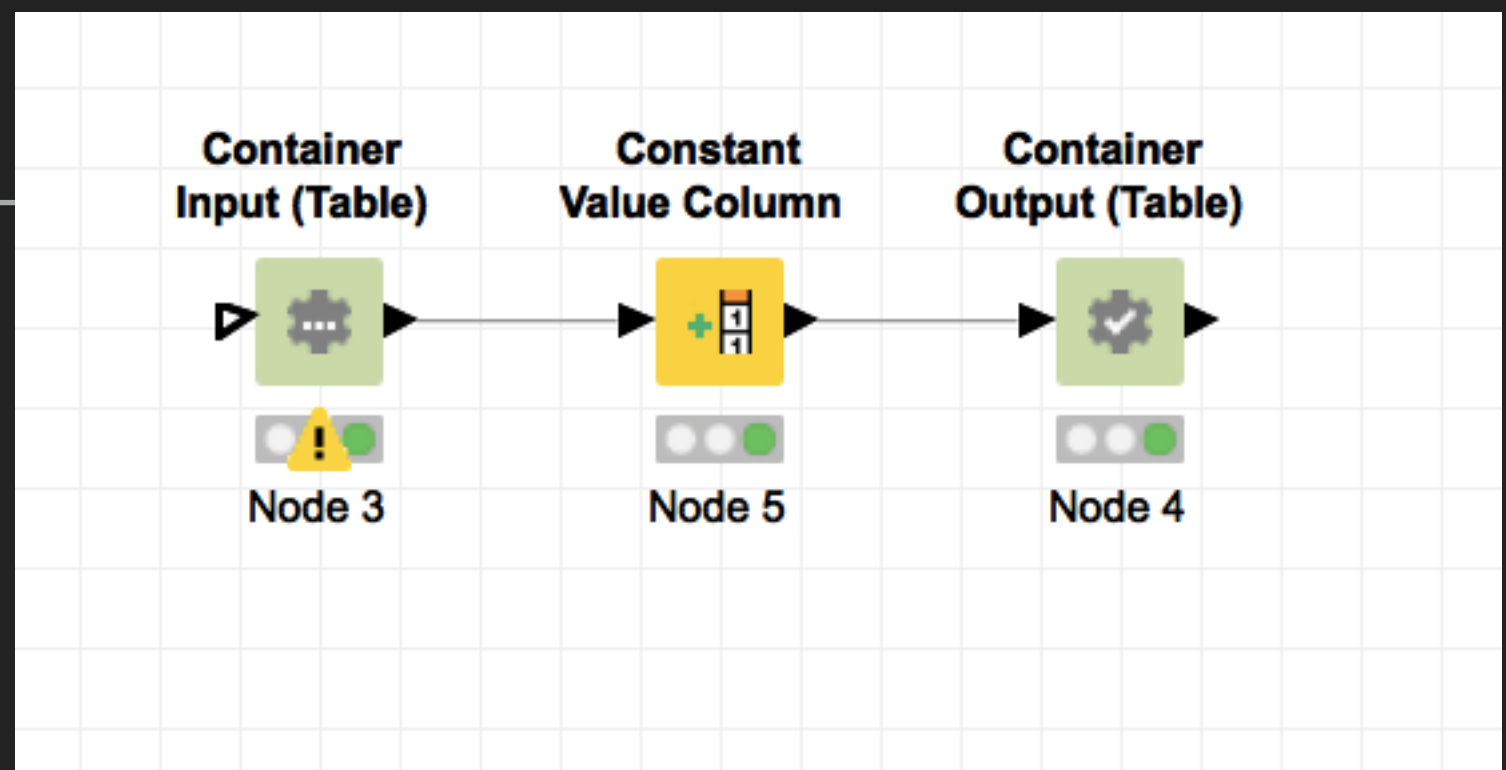
Project description

Utilities for working with KNIME workflows and data.

Via the Workflow class, a KNIME Workflow can be run via KNIME's batch executor (requires KNIME be installed on the local system). Inputs to the "Container Input (Table)" nodes in a KNIME Workflow can be supplied as either Python dicts or pandas DataFrames. Likewise, outputs captured from "Container Output (Table)" nodes are provided back as either Python dicts or pandas DataFrames.

ポイント

- ▶ knime.py
- ▶ データセットの受け渡しは、pandas
 - ▶ KNIME側は、Container Input(Table)で受け取り、
 - ▶ Container Output(Table)で受けわたす



2019.09.21

```
1  from flask import Flask
2  import pandas as pd
3  import knime
4  import os
5
6  knime.executable_path = "/Applications/KNIME 4.0.1.app/Contents/MacOS/Knime"
7  WORKSPACE = "/Users/chemoinfo/knime-workspace"
8  app = Flask(__name__)
9
10 @app.route("/")
11 def hello():
12     workflow = "AUTOMATION/sample0"
13     input_table_1 = pd.DataFrame(
14         [ ["blau", -273.15], ["gelb", 100.0]], columns=["color", "temp"])
15
16     with knime.Workflow(workflow_path=workflow, workspace_path=WORKSPACE) as wf:
17         wf.data_table_inputs[0] = input_table_1
18         wf.execute()
19         output_table = wf.data_table_outputs[0]
20
21     return output_table.to_html()
22
23 if __name__ == "__main__":
24     app.run( debug=True )
```