Jupyter notebooks: How do kernels work internally?

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About me

- PhD student in Materials Theory at ETH Zürich
- Python/Jupyter notebooks are my workhorse for everything around large-scale quantum-mechanical simulation programs
- Likes to teach – SWC workshops, workshops in my research area, …

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Kernel Restarting

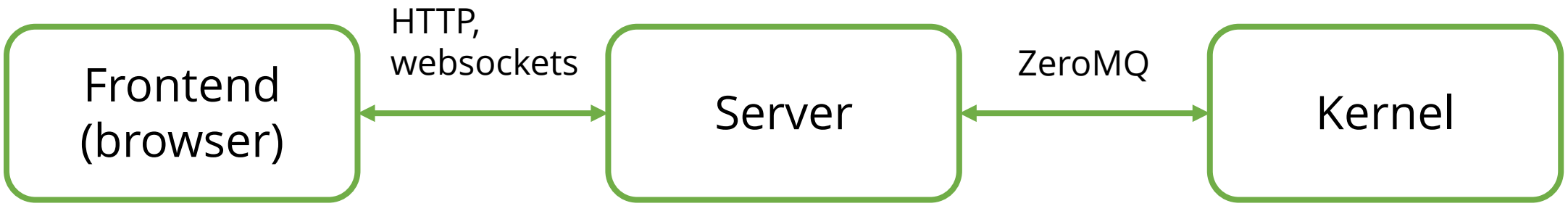
The kernel appears to have died. It will restart automatically.

OK

IPython vs. Jupyter

- Since version 4.0: Split between ipython and jupyter
- IPython: Provide a “more usable” python environment for interactive work
  - REPL and kernel mode
  - Environment on top of a python interpreter, such as CPython, PyPy, ..
- Jupyter: Client/server infrastructure, can use ipython as one possible kernel

Architecture of Jupyter



How does the server know about available kernels?

- KernelManager reads JSON files with kernelspec:

```
$ jupyter kernelspec list
Available kernels:
python3         /Users/thoelef/anaconda3/lib/python3.6/site-packages/ipykernel/resources
ir              /Users/thoelef/Library/Jupyter/kernels/ir
julia-0.4       /Users/thoelef/Library/Jupyter/kernels/julia-0.4
python2         /Users/thoelef/Library/Jupyter/kernels/python2
scala211        /Users/thoelef/Library/Jupyter/kernels/scala211
```

- nb_conda_kernels replaces the standard KernelManager with a custom one that “emulates” kernel confs for all conda environments

Example of KernelSpec file

- Usually, executes python program, but can be any other program that implements the messaging protocol

```
{
    "display_name": "Julia 0.4.5",
    "argv": [
        "/Applications/Julia-0.4.5.app/Contents/Resources/julia/bin/julia",
        "-i",
        "-F",
        "/Users/thoelef/.julia/v0.4/IJulia/src/kernel.jl",
        "{connection_file}"
    ],
    "language": "julia”
}
```

The connection file contains the sockets used for communication


```
{
 "shell_port": 63454,
 "iopub_port": 63455,
 "stdin_port": 63456,
 "control_port": 63457,
 "hb_port": 63458,
 "ip": "127.0.0.1",
 "key": "c78c3588-0ab3-408c-8bc3-55b9cd9ee291",
 "transport": "tcp",
 "signature_scheme": "hmac-sha256",
 "kernel_name": ""
 }
```

Jupyter message protocol

Messages are sent on five channels:

```
{
 'header' : dict,
 'msg_id' : str,
 'msg_type' : str,
 'parent_header' : dict,
 'content' : dict,
 'metadata' : dict,
}
```

- Shell
- Control
- IOPub
- stdin
- heartbeat

http://jupyter-client.readthedocs.io/en/latest/messaging.html

How to implement a custom kernel

- Write from scratch, have to start at socket level to send/receive messages
  - Can be done in any language

- Use ipython module that takes care of communication
  - Good if python as base layer works
  - Can be used to control REPLs

Live demo!

Examples of languages for which kernels are written

- IJulia, R, PySpark, JavaScript, Matlab, …
- C, Fortran, C#, Scala, …

https://github.com/jupyter/jupyter/wiki/Jupyter-kernels

https://github.com/dsblank/simple_kernel

https://github.com/QuantStack/xeus

Summary

- Versatile architecture of Jupyter allows custom kernels for a variety of languages
- Effort to support a new language low when it can be controlled from python (pexpect), higher when implemented from scratch in native language