USPAS – *Simulation of Beam and Plasma Systems*

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Computer Lab:     Computational Reproducibility

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*radiasoft*

U.S. Particle Accelerator School  sponsored by **Old Dominion University**

http://uspas.fnal.gov/programs/2018/odu/courses/beam-plasma-systems.shtml

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**U.S. DEPARTMENT OF**
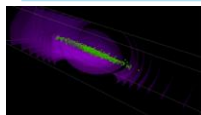**ENERGY**
Office of Science

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## Goals

- Familiarize yourself with the Jupyter hub server
  - browser-based terminal window with bash
  - many particle accelerator codes pre-installed (on RadiaSoft server)
  - supports Jupyter (aka IPython) notebooks

- Explore use of a Jupyter notebook for particle accelerator simulations
  - assume you are asked to do space charge simulations with Synergia
    - https://web.fnal.gov/sites/Synergia/SitePages/Synergia%20Home.aspx
    - http://compacc.fnal.gov/~amundson/html/   (draft user manual)
  - typically, you must do the following:
    - **find the source repository, download, install**
    - **learn how to run the code, then visualize the output**
  - if someone provides you with a well-written Jupyter notebook…
    - **then you can start working immediately**

- Consider expansion of a 2D (i.e. very long) proton beam in a drift
  - this is an important exercise with any particle tracking code

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### Beam dynamics with space charge via Synergia 2.1

Synergia: A comprehensive accelerator beam dynamics package
http://web.fnal.gov/sites/synergia/SitePages/Synergia%20Home.aspx

**Fermilab**
Accelerator Simulation Group

Computer time from INCITE

**INCITE**
U.S. DEPARTMENT OF ENERGY
LEADERSHIP COMPUTING

James Amundson,  Qiming Lu,
Alexandru Macridin,  Leo Michelotti,
Chong Shik Park,  (Panagiotis Spentzouris),
Eric Stern  and  Timofey Zolkin

The ComPASS Project
High Performance Computing for Accelerator Design and Optimization
https://sharepoint.fnal.gov/sites/compass/SitePages/Home.aspx
Funded by DOE SciDAC

**CAMPA**   Consortium for Advanced Modeling of Particle Accelerators
Funded by DOE
**Fermilab**

Slide courtesy of James Amundson | Advancing Particle Accelerator Science with High Performance Computing        11/12/15

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### JupyterHub (Part 1)

Jupyter & JupyterHub, http://jupyter.org
RadiaSoft, https://uspas-jupyter.radiasoft.org

**jupyterhub**

- Create a GitHub account (if necessary),  https://github.com
- Go to the RadiaSoft server,  https://uspas-jupyter.radiasoft.org
- Authorize the server with your GitHub credentials
  - it can verify your identity and provide a persistent simulation workspace
  - the server saves your GitHub username, but never sees your password
    - **RadiaSoft only uses your username to identify you on the Jupyter server**

- Upon first login, you might see:

- If so, just select 'My Server'
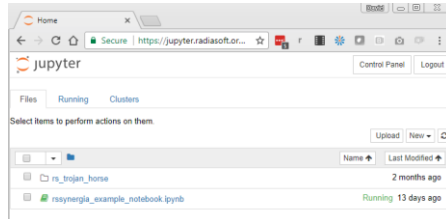  - activates your instance
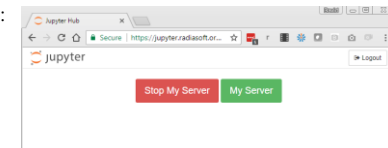
## *JupyterHub* (Part 2)

- Next you'll see something like the following, but with no files:



- To upload a Jupyter notebook, or any file, click on the 'Upload' button.

- To create a subdirectory, click on the 'New' button, then select 'Folder'.

- To rename, delete or move a file or folder, select the box to its left
  – causes necessary buttons to appear in the upper-left region of your browser

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## *JupyterHub* (Part 3)

- For a bash terminal, click on the 'New' button and select 'Terminal'
  – the terminal window will open in a new tab of your browser
  – it will looking something like this:



  – it's like any bash terminal
    • **but you don't have X11**
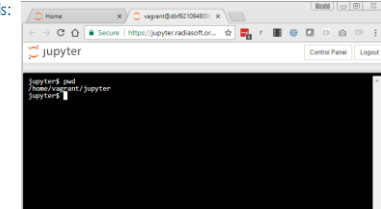
- The working directory is   /home/vagrant/jupyter/
  – everything uploaded via the JupyterHub interface appear in that directory
  – you are free to 'cd' upward and create other directories
  – you can also 'scp' files to/from other computers
  – you can 'git pull' repos from wherever you like

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## *Pull a Jupyter notebook from GitHub*

- Type the following in your terminal window:

```
jupyter$ cd /home/vagrant/jupyter

jupyter$ git clone \
> https://github.com/radiasoft/rssynergia.git

jupyter$ mkdir uspas

jupyter$ cp \
> rssynergia/examples/drift_expansion/sc_drift_expansion.ipynb \
> uspas/

jupyter$ cp \
> rssynergia/examples/drift_expansion/myGaussianBunch.txt \
> uspas/
```

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## *Run Synergia from a Jupyter notebook*

- Go back to the main browser tab for the JupyterHub server
  – click on the directory named  'uspas'
  – click on the file named  'sc_drift_expansion.ipynb'
  – this opens a Jupyter notebook in a new browser tab
- Type 'shift enter' repeatedly to advance through the notebook
  – pause at each cell to read the docs or look over the code
  – if you see an asterisk in the square brackets to the left…
    • **that means the Python kernel is working**
    • **wait until a number replaces the asterisk;  look for any output**
- Once you understand what's happening, scroll back to the top
  – click on 'Kernel' and then select 'Restart & Clear Output'
  – this prevents a lot of problems, when starting a new Synergia simulation
- Find the discussion of drift length in the 4$^{th}$ cell
  – in the cell above, modify this Python code
    `opts.add("turns",30,"Number of turns", int)`
  – to specify 60 "turns", so that the drift length is increased to 6 m
- Click on 'Cell' and then select 'Run All'
  – wait for the simulation to complete, then observe the results

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### *Your Tasks for this afternoon*

- Save the final plot for at least 3 different propagation distances
  - put these plots into a form (or location) that can be shared later
- For one choice of propagation distance, choose two new currents
  - put these 3 plots into a file (or location) that can be shared later
  - make sure the curve labels and plot title are correct for each plot
- For one choice of current and propagation distance
  - increase the Synergia step size repeatedly (keep distance constant)
  - look for signs of problems due to poor resolution
  - make at least 3 plots, with meaningful titles

- Homework for this evening:
  - Write a paragraph for each of your 3 sets of plots
  - Explain what you did and/or what you learned
  - Feel free to comment on the Jupyter notebook experience
  - Make plots and text available to instructors (print, PDF, web…)