## Introduction to Interactive HPC

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## What is Interactive Computing?

Interactive Computing is about immediacy. When the human requests an action, the computer immediately responds. When the computer finishes a task, the human immediately perceives the result.

- Software GUIs
- Prototyping workflows
  - Design your workflow for a single node (multi-core) or small set of nodes
  - Discover and test new tools/concepts
  - Profile, optimize and debug
- Data Visualization



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## Why Interactive HPC?

### HPC is part of a larger research workflow

### Dr. so-and-so needs to explore a huge dataset

Needs: interactivity, analytics tools, large memory/storage

## **Dr.** such-and-such is preparing to create a cutting-edge simulation visualization

Needs: interactivity, remote visualization, compute, bandwidth

### A grad student is prototyping a new algorithm

Needs: interactivity, dev and debug tools, time to iterate

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## **Tutorial Outline**

- Batch vs. Interactive Computing @ MSI
- Getting Started with Interactive Resources
  - Connecting to MSI
  - Conscientious Computing
  - Prototyping Workflows
- Hands-on
  - Remote desktops
  - Jupyter Notebooks



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#### Researcher

Needs compute resources

#### **Secure Network**

On-campus eduroam or ethernet Off-campus via UMN VPN

#### **MSI Access Gateway**

OnDemand Portal SSH Command Line Other Web Portals

#### **HPC Compute**

Computation on MSI clusters Agate, Mangi, Mesabi

#### **Data Storage**

Primary - Home+Project Dirs 2nd Tier - object storage Scratch storage areas

### MSI Access Overview

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### **Resource Allocations**

ALL groups will have access to these basic resources:

- High Performance Computing cluster access
- High Performance Storage
  - 150 GB home directory quota or more if requested
  - Home and project storage accessible from most MSI systems
- Access to interactive gateways
- Access to MSI labs
  - contact us to activate your Ucard for physical access

### Survey of Options

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## Batch Jobs

- When should you use Batch Jobs?
  - Whenever possible! This is the traditional way to work in HPC
  - Share resources and be considerate of other researchers
- What are the benefits of Batch Jobs?
  - Headless execution of automated processes
  - Long runtimes
  - Large core counts
  - A scheduler packs jobs in hardware to maximize utilization, reduce latency, etc.

## Interactive Options

- → OnDemand Portal
- → Interactive batch (srun via the command line)
- → Jupyter portal (sharable reproducible computing)

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- → Galaxy portal (graphically compose workflows)
- → Specialized solutions
  - CITRIX for Windows apps
  - Stratus "private cloud" instances



### **OnDemand Portal**

https://ondemand.msi.umn.edu

- OnDemand Web Portal is a new offering in 2022
- One-stop access portal for interactive HPC services
  - Remote desktop access
  - Command line terminal
  - > File browser
  - Launchers for common GUI scientific applications
  - > JupyterLab server access
  - > RStudio server access







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## Interactive Command Line

### ssh <username>@<resource>.msi.umn.edu

### See: <a href="https://www.msi.umn.edu/content/connecting-hpc-resources">https://www.msi.umn.edu/content/connecting-hpc-resources</a>

- → SSH is the traditional first point of access to MSI resources
- → Access agate mesabi or mangi
- → Uses ssh program available on most personal computers

These "login nodes" are shared by many MSI users. They are NOT for heavy computational tasks. Appropriate uses include:

- Browsing and editing files
- ✓ Submitting jobs
- Querying job status and other informational commands
- Browsing software modules
- ✓ *Light* testing or software compilation

| C:\Users\                                    | ssh landw020@mangi.msi.umn.edu   |  |  |  |  |  |  |
|--|--|--|--|--|--|--|--|
| Password:<br>Last login:                     | Wed Feb 10 15:06:20 2021 from x-10-21-31-220.vpn.umn.edu   |  |  |  |  |  |  |
|  | University of Minnesota Supercomputing Institute   |  |  |  |  |  |  |
|  | University of Minnesota Supercomputing Institute<br>Mangi<br>AMD EPYC Linux Cluster  |  |  |  |  |  |  |
| For assistan<br>help@msi.umn                 | ce please contact us at https://www.msi.umn.edu/support/help.html<br>.edu, or (612)626-0802.   |  |  |  |  |  |  |
| Home directo<br>your home di<br>available in | ries are snapshot protected. If you accidentally delete a file in<br>rectory, type "cd .snapshot" then "ls -lt" to list the snapshots<br>order from most recent to oldest. |  |  |  |  |  |  |
| January 6, 2                                 | 021: Slurm is now the scheduler for all nodes.   |  |  |  |  |  |  |
| landw020@ln1                                 | 002 [~] %  |  |  |  |  |  |  |

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### Interactive Batch with 'srun'

srun <resource requests> --pty bash

See: <u>https://www.msi.umn.edu/content/interactive-queue-use-srun</u>

- Dedicated compute resources via the scheduler
- → Command line terminal running on the cluster
  - similar to a SSH session
- → Supports all usual Slurm options and commands
- → Best used with interactive partitions
  - have priority access for small interactive job requests
- Job terminates when shell exits or connection broken

### Example:

srun -N 1 --ntasks-per-node=4 --mem-per-cpu=1gb -t 1:00:00 -p interactive --pty bash

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## Jupyter Notebooks Portal

### https://notebooks.msi.umn.edu

See:

https://www.msi.umn.edu/support/faq/how-do-i-get-started-jupyter-notebooks

- → JupyterLab web-based computational workspace
- → Jupyter Notebook document-oriented computing
- Python and R support provided, users can install additional languages/environments
- → Integrated terminal, file editing and browsing
- → Runs via scheduler, multiple resource options available
- → Session persists until time expires or manually shut down



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## Web Portals: Galaxy

### http://galaxy.msi.umn.edu

Galaxy is a web-based workflow manager, principally for bioinformatics/'omics research

- → Compose data analysis workflows in a unified data flow view
- → Workflows execute when requested on MSI compute clusters
- → Wide variety of bioinformatics and 'omics applications available as tools

#### See

https://www.msi.umn.edu/content/galaxy for additional details, especially regarding linking data into Galaxy

|   |              | alaxy.msi. | umn.edu   | Ċ                  | ; 100+   |  |  |
|---|--------------|------------|---|--------------------|--|--|--|
| 🗧 Galaxy / UMN  | Analyze Data | Workflow   | Shared Data 😽 Vi  | isuali             | zation - Help - User -   |  |  |
| Tools   | Workflow Can | vas   Test | (   | \$                 | Details  |  |  |
| Tools          search tools         Get Data         Send Data         Lift-Over         Text Manipulation         Filter and Sort         Join, Subtract and Group         Convert Formats         Extract Features         Fetch Sequences         Fetch Alignments         Get Genomic Scores         Operate on Genomic Intervals         Statistics         Wavelet Analysis | Workflow Can | ataset :   | Filter SAM or BAM<br>SAM or BAM File to<br>Output alignments<br>regions in the BED<br>output1 (sam, ban | p Fil<br>FIL<br>n) | Details         Filter SAM or BAM files on         FLAG MAPQ RG LN or by region         (Galaxy Tool Version 1.1.1)         SAM or BAM File to Filter         Data input 'input1' (sam or bam)         Header in output         Include Header         Minimum MAPQ quality score         Filter on bitwise flag         no         Select alignments from Library |  |  |
| Graph/Display Data<br>Graph/Display Data<br>Regional Variation<br>Multiple regression<br>Multivariate Analysis<br>Evolution<br>Motif Tools<br>Multiple Alignments<br>Metagenomic analyses<br>FASTA manipulation<br>C  |              | 8          |   | P)                 | Requires headers in the input SAM or<br>BAM, otherwise no alignments will be<br>output.<br>Select alignments from Read Group<br>Requires headers in the input SAM or<br>BAM, otherwise no alignments will be<br>output.  |  |  |

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## Need Windows?

MSI no longer provides Windows application servers.

Select HPC applications that require Windows are available through partnership with OIT via CITRIX

See:

www.msi.umn.edu/support/faq/how-do-i-connect-citrix-wi ndows-virtual-machine for access to Apps.umn.edu







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#### **MSI Access Gateway**

OnDemand Portal SSH Command Line Other Web Portals

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### Pre-requisites to connect

### Campus VPN

https://it.umn.edu/services-technologies/virtual-private-network-vpn

- → MSI services are only available to on-campus network addresses
- → Especially during the pandemic, many users are working off-campus
- → VPN clients and instructions are available from OIT for most operating systems and mobile devices

### **DUO Authentication**

https://it.umn.edu/services-technologies/self-help-guides/duo-set-use-duo-security

- → DUO 2-factor authentication is required for most MSI services
- → DUO is also required to connect to the campus VPN



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## Sidebar: Windows SSH and File Transfer

Current Windows 10+ computers will have ssh/scp available from the Windows terminal.

For users who desire a graphical ssh or file transfer client: <u>https://winscp.net/eng/downloads.php</u>

### Download and install both WinSCP and PuTTY\*

\*MSI recommends WinSCP and PuTTY for Windows users, but does not offer support for these programs. Contact your local IT department for assistance.

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## Choosing a Cluster/Partition

See: <a href="https://www.msi.umn.edu/content/choosing-job-partition">https://www.msi.umn.edu/content/choosing-job-partition</a>

- Long running jobs and batch jobs run on Agate/Mesabi/Mangi
- MSI compute clusters are heterogeneous (e.g., up to 1TB Memory, GPUs, SSDs, etc.)
  - > **Think**: match your needs to available configurations
    - Do: reserve the (CPU/RAM/GPUs/etc) that you need
    - Avoid: reserving much more (waste, long queue times) or less than required (job doesn't finish before walltime expires)

For interactive use, begin with the **interactive** partition and experiment from there.

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## Interactive Services OnDemand

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Open OnDemand Files Jobs Clusters Interactive Apps

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OnDemand provides an integrated, single access point for all of your HPC resources.

#### Message of the Day

Open OnDemand is a web-based portal for interactive access to MSI's compute clusters. You can access your MSI files, view your current jobs on the MSI clusters, and access a command line or interactive desktop on a cluster compute node, with configurable memory and compute resources. You also have access to a set of familiar servers, interactive development environments, and graphical user interfaces that have been adapted to use the Open OnDemand platform.

For more information about Open OnDemand at MSI, please visit https://www.msi.umn.edu/content/using-openondemand

For assistance please contact us at https://www.msi.umn.edu/content/helpdesk, help@msi.umn.edu, or (612)626-0802.

### https://ondemand.msi.umn.edu/

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Open OnDemand Files - Jobs - Clusters - Interactive

Interactive Apps -

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### Services accessed through menu bar

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For more information about Open OnDemand at MSI, please visit https://www.msi.umn.edu/content/using-openondemand

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| Open OnDemand             | Files -     | Jobs <del>-</del> | Clusters *            | Interactive Apps -                                     | My Interactive Sessions  |   |
|---------------------------|-------------|-------------------|-----------------------|--|--|---|
|                           |             |                   | >_Agate S<br>>_Mesabi | Shell Access<br>Shell Access<br>hand line<br>al access | Command line terminal:<br>- "SSH" in a web bro<br>- Launch terminal on<br>- Roughly equivalent<br>ssh <username>@ag<br/>- Also launch in spec<br/>file browser pane</username> | wser (almost)<br>a cluster headnode<br>t to e.g.<br>gate.msi.umn.edu<br>cific directory via |
| ↑ home / support / millig | an / 🕼 Char | >_ Open in Terr   | ninal 🕨 🕂 New File    | Rew Directory  | ★ Download Copy/Move Delete          Copy path   |   |

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| Open OnDemand Files - Jobs - Clusters -                               | Interactive Apps 🚽 🖻 My Interactive Sessions  |
|---|---|
|   | Desktops<br>Desktop Persistent Desktop  |
| Interactive Apps menu<br>lists available application<br>launchers     | GUIs<br>ANSYS Workbench   |
| Each launcher leads to a session options page                         | MATLAB  |
| Each session runs as an interactive job on a cluster resource         | <ul> <li>Abaqus</li> <li>COMSOL Multiphysics</li> <li>IDL</li> <li>Mathematica</li> </ul> |
| Launchers also available<br>via the Interactive<br>Sessions dashboard | Servers<br>≝ Jupyter<br>◆ RStudio Server  |

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#### Home / My Interactive Sessions / Jupyter

| Interactive Apps    | Jupyter                    |
|---------------------|----------------------------|
| Desktops            | This app will launch a Ju  |
| ₽Desktop            | Cluster                    |
| Persistent Desktop  | agate                      |
| GUIs                | Jupyter interface          |
| ANSYS Workbench     | Lab                        |
| iii IGV             | This defines the interface |
| ▲ MATLAB            | Jupyter Python             |
| IDEs                | MSI Python 3.8.3 / Jup     |
| 📥 Abaqus            | This defines the Python d  |
| COMSOL Multiphysics | Account                    |
| M IDL               | Resources                  |
| Mathematica         | Interactive - 2 cores, 32  |
| Servers             | Time Limit                 |
| S Jupyter           | 4 Hours                    |
| RStudio Server      | Shorter times will probabl |
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| ant to start.         |

I would like to receive an email when the session starts

Launch

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### Example launcher: Jupyter server

Options to customize most aspects of the interactive job

- cluster / partition
- group (if multiple available)
- resource requests
- launcher-specific parameters (e.g. Python environment for Jupyter servers)

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Open OnDemand Files -

Jobs ▼ Clusters ▼ Interactive Apps ▼



#### **Session cleanup**

OnDemand sessions run as scheduled jobs: cancel jobs or use desktop "logout" to end jobs and release resources early, or allow them to close automatically when walltime expires

Logging out from this page clears browser login but otherwise has no effect on active OnDemand sessions

Rarely may need to use "restart server" option to recover from failures

Logout and server restart options

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# Interactive Jobs with **srun**

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## Selecting Resources

- SSH to any cluster headnode:
  - ssh <username>@agate.msi.umn.edu Or
  - ssh <username>@mesabi.msi.umn.edu or

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- Launch interactive terminal in OnDemand
- Queue an Interactive job on the cluster:
  - srun <job options> --pty bash

## Selecting Resources

Options to srun specify job requirements:

- **srun** [options]
  - --time=8:00:00 job can run for up to 8 hours
  - -N 1 --cpus-per-task=4 job requests 4 CPUs on one node
  - --mem=2500m job requests 2500 MB (2.5GB) of RAM
  - -p interactive
  - --pty bash job must specify shell program to run
- Enable graphics via X-tunneling (--x11)
  - not available in web terminals (OnDemand, Jupyter, etc)

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## Selecting Resources

Example - basic interactive session with 4 CPU cores, 8 GB RAM, 4 hours runtime:

srun -N 1 --ntasks-per-node=4 --mem-per-cpu=1gb -t 1:00:00 -p interactive --pty bash

Example - interactive session for machine learning with 1 A40 GPU, 12 CPU cores, 1 hour runtime:

srun -n 12 -t 1:00:00 -p interactive-gpu --gres=gpu:a40:1 --pty bash





## Software Modules

See: https://www.msi.umn.edu/content/accessing-software-resources

- See all modules available
  - module avail
- Load a module (adds commands to your shell)
  - module load python3
- Run the software from the module

# Mail Terminal 1 X milligan@cn0060 [~] % module avail python ------ /panfs/roc/soft/modulefiles.hpc ---python/3.7.1\_anaconda python3/3.7.1\_anaconda python2/2.7.15\_anaconda

------ /panfs/roc/soft/modulefiles.common --python/3.2.3 python/3.4 python/3.6.3(default) python2/2.7.12\_anaconda4.1.1 python2/2.7.12\_anaconda4.2(default) python2/2.7.16\_anaconda2019.10 python3/3.4 python3/3.5.2\_anaconda5.0.1(default) python3/3.6.3\_anaconda5.0.1(default) python3/3.7.4\_anaconda2019.10 python3/3.8.3\_anaconda2020.07\_mamba

• ipython



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## Optional: SSH Keys

- SSH keys allow terminal logins without typing a password repeatedly
- Some applications may automatically make SSH connections and may require SSH keys
- See: <u>www.msi.umn.edu/support/faq/how-do-i-setup-ssh-keys</u>





## Clean up your session

- Delete the session (choose one)
  - Exit out of all connections
  - scancel <job ID>
- What happens on disconnect/delete?
  - All computation stops
- How to resume?
  - Start from zero; or load intermediate files (if you created them)



### Interactive Linux Desktops

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| •     | k     | onsole.deskt<br>op |  |       |   |
| 8     |       |                    |  |       |   |

Interactive desktop: noVNC session proxied through OnDemand server

Graphical fidelity will suffer on low-bandwidth connections but quality can be adjusted to maintain usability

Good connections allow graphically intensive apps, GPU accelerated graphics available on GPU nodes

Session persists until logged out on desktop - don't forget to log out to release resources when done!

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## Session Clean-up and Resume

- What is lost when the connection drops?
  - Instance: if not expired, reconnect to the same Instance
  - Data: no loss
- What if you Logout?
  - Instance: Terminated; Reconnect and start fresh
  - Data: Scratch data is deleted periodically\* (clean up after yourself to be sure); No loss for data in group home
- How do you reconnect?
  - Login again through OnDemand Interactive Sessions dashboard



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Hands-On: Interactive Development and Data Interrogation with Jupyter

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## Start your Jupyter Session



- Visit <u>notebooks.msi.umn.edu</u>
- Select the default interactive job
- There will be a short wait while the background job starts running
- When ready, the JupyterLab workspace will load in your web browser window



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## JupyterLab Workspace

### See: https://jupyterlab.readthedocs.io/en/stable/user/interface.html

- → Rich tabbed multi-document workspace
- → File navigation able to access home and group directories
- → Reproducible, sharable computational stories in Jupyter Notebooks
- → View and edit text and other files directly in JupyterLab
- → Command line terminal available

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| œ                   | 📶 bar.vl.json             | 9 minutes ago           | Tn [5]:      | 1                            | import n  | andas       |              |             |                                      |  |                                   |
| 0                   | Dockerfile                | 5 months ago            | 211 [0]1     | 2                            | <pre>df = pandas.read_csv('/data/iris.csv') df.head(20)</pre> |             |              |             | JupyterLab: The next generation user |  |                                   |
| 2                   | iris.csv                  | 6 months ago            |              | 3                            |   |             |              |             | interface for Project Jupyter        |  |                                   |
|                     | (:) japan_meterological_a | ological_a 5 months ago | 5 months ago | 0.4[5].                      |   |             |              |             |                                      | https://github.com/jupyter/jupyterlab  |                                   |
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| 0                   | M README.md               | 5 months ago            |              | 0                            | 5.1   | 3.5         | 1.4          | 0.2         | se                                   | it has been a conaboration between.  |                                   |
| Zika_assembled_geno | zika_assembled_geno       | 5 months ago            |              | 1                            | 4.9   | 3.0         | 1.4          | 0.2         | setosa                               | <ul> <li>Project Jupyter</li> </ul>  |                                   |
|                     |                           |                         |              | 2                            | 4.7   | 3.2         | 1.3          | 0.2         | setosa                               | Bloomberg  |                                   |
|                     |                           |                         |              | 3                            | 4.6   | 3.1         | 1.5          | 0.2         | setosa                               | Anaconda   |                                   |
| aus                 |                           |                         |              | 4                            | 5.0   | 3.6         | 1.4          | 0.2         | setosa                               | 1) Building blocks of  |                                   |
|                     |                           |                         |              | 5                            | 5.4   | 3.9         | 1.7          | 0.4         | setosa                               | interactive computing  |                                   |
|                     |                           |                         |              |                              | 6   | 4.6         | 3.4          | 1.4         | 0.3                                  | setosa   | 🔀 bar.vl.json 🛛 🔀 1024px-Hubble 🖓 |
|                     |                           |                         |              | 7                            | 5.0   | 3.4         | 1.5          | 0.2         | setosa                               |  |                                   |
|                     |                           |                         |              | 8                            | 4.4   | 2.9         | 1.4          | 0.2         | setosa                               | 1 de hai   |                                   |
|                     |                           |                         |              | 9                            | 4.9   | 3.1         | 1.5          | 0.1         | setosa                               |  |                                   |
|                     |                           |                         |              | 10                           | 5.4   | 3.7         | 1.5          | 0.2         | setosa                               |  |                                   |
|                     |                           |                         |              | 11                           | 4.8   | 3.4         | 1.6          | 0.2         | setosa                               | Participation of Friday  |                                   |
|                     |                           |                         |              | 12                           | 4.8   | 3.0         | 1.4          | 0.1         | setosa                               | X  |                                   |
|                     |                           |                         |              | 13                           | 4.3   | 3.0         | 1.1          | 0.1         | setosa                               |  |                                   |
|                     |                           |                         |              | 14                           | 5.8   | 4.0         | 1.2          | 0.2         | setosa                               | The second s |                                   |

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## Jupyter Cleanup





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## Additional Documentation

- Overview of IPython's architecture for parallel and distributed computing.
- Detailed discussion of IPython cluster controller and engines.
- Discussion of IPython magic commands
- Official IPython documentation





These slides and the hands-on guide will be posted to <a href="http://msi.umn.edu">http://msi.umn.edu</a> (see the "MSI Tutorials" section)

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