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Waterview Conference Center, Arlington, VA

Cloud Computing Clusters for Scientific Research*

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Challenge of NSF Grant

- Complete scientific computing cloud environment: for materials science, robust, easy to use

Goals of CC for Scientific Computing*

- On-demand access without the need to purchase, maintain, or understand HPCs
- Optimized/pre-installed HPC scientific codes
- Low cost HPC access to a wide class of scientists

*J. J. Rehr, F. Vila, J. P. Gardner, L. Svec and M. Prange
CiSE May/June 2010

The Target Scientific CC User

- Not usually HPC “gurus”:
  - Little experience with parallel computing, code compilation & optimization, etc.
  - Limited access to HPC resources

- “Would rather be doing science...”

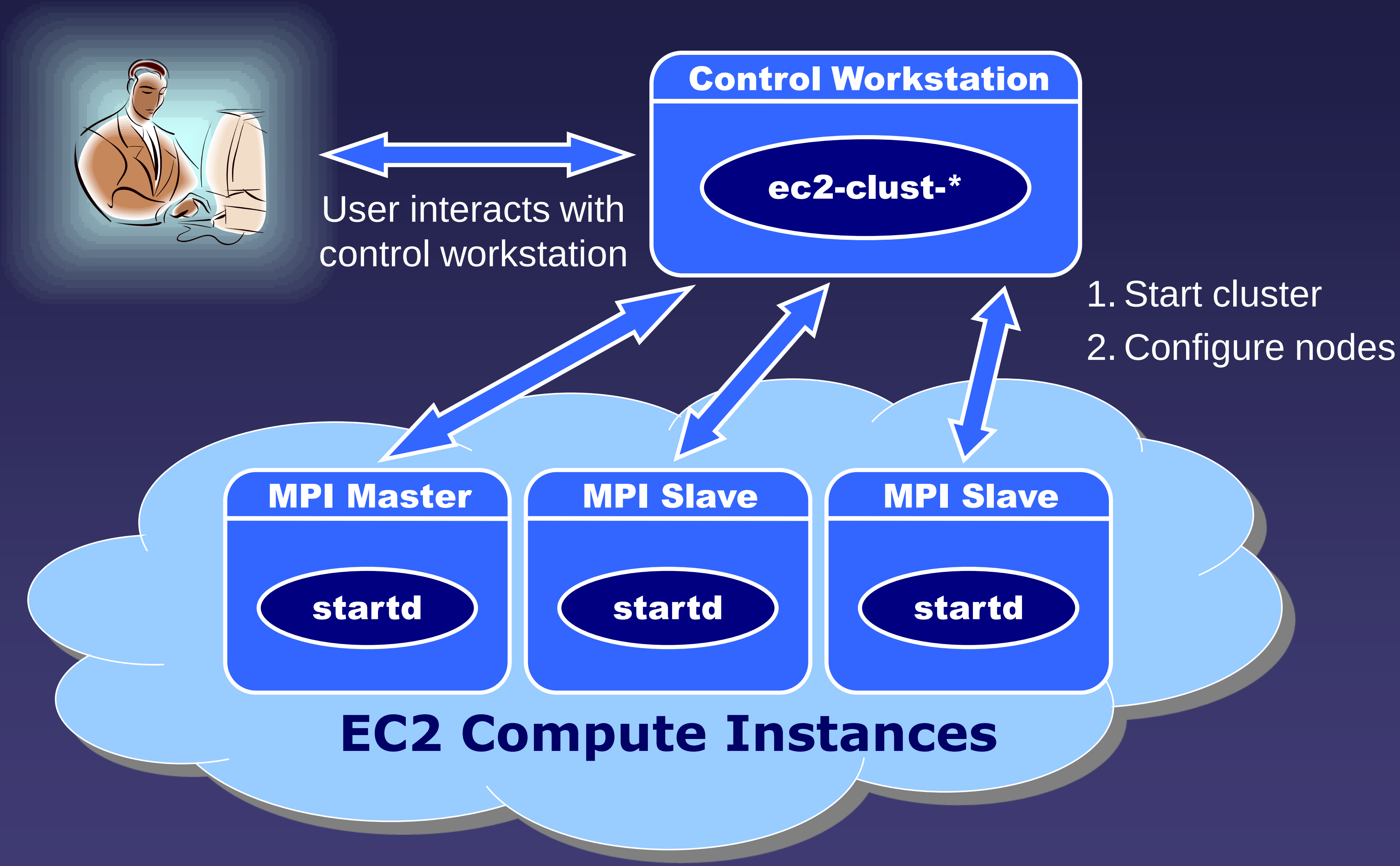
Scientific Cloud Computing Programming Philosophy

- Preserve current HPC paradigm (MPI) on the cloud
- Simplify access to HPC for a broad user base

Development Strategy

1. Develop AMIs (Amazon Machine Images) for HPC scientific applications in materials science
2. Develop shell-scripts that make the EC2 look & run like a local HPC cluster: ”virtual supercomputer on a laptop”
3. Test serial, parallel & network performance
4. Develop GUI to control/run codes & I/O

Cloud→Cluster with UW Cluster tools*



User interacts with control workstation

Control Workstation

ec2-clust-*

1. Start cluster

2. Configure nodes

MPI Master

startd

MPI Slave

startd

MPI Slave

startd

EC2 Compute Instances

* http://www.phys.washington.edu/feff/scc

UW EC2 Cluster Tools

UW EC2 tools on local control machine

Name	Function	Analog
ec2-clust-launch *N*	Launches cluster with N instances	boot
ec2-clust-connect	Connect to a cluster	ssh
ec2-clust-put	Transfer data to EC2 cluster	scp
ec2-clust-get	Transfer data from EC2 cluster	scp
ec2-clust-list	List running clusters	
ec2-clust-terminate	Terminate a running cluster	shutdown

The tools hide a lot of the “ugliness”:

```
ec2-clust-connect
```

```
ssh -i/home/fer/.ec2_clust/.ec2_clust_info.7729.r-de70cdb7/key_pair_fdv.pem feffuse@ec2-72-44-53-27.compute-1.amazonaws.com
```

Current EC2 AMIs

- New 32-bit and 64-bit AMIs
- Amazon’s HPC “cluster instance”
- EBS backed instances (faster disk access/boot time)

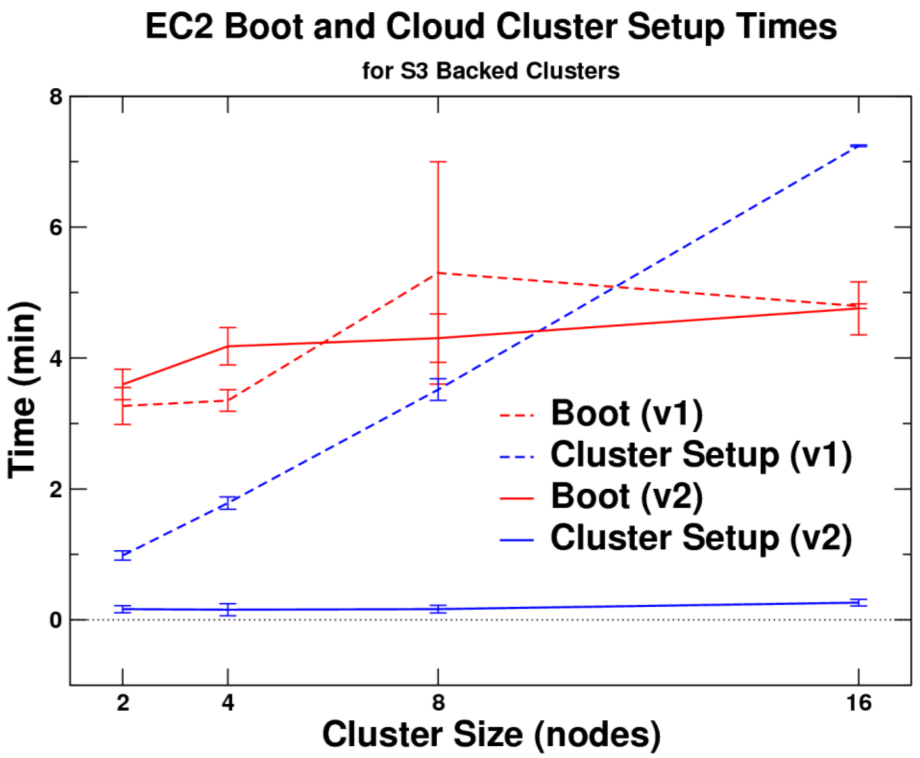
- Several Condensed Matter/Materials Science Codes:
  - X-ray Spectroscopy: FEFF9, IFEFFIT
  - Electronic Structure: WIEN2k, ABINIT, Quantum Espresso
  - Excited States: AI2NBSE, OCEAN, Exc!ting, RT-SIESTA

UW CC Tools: 2nd generation (v2)

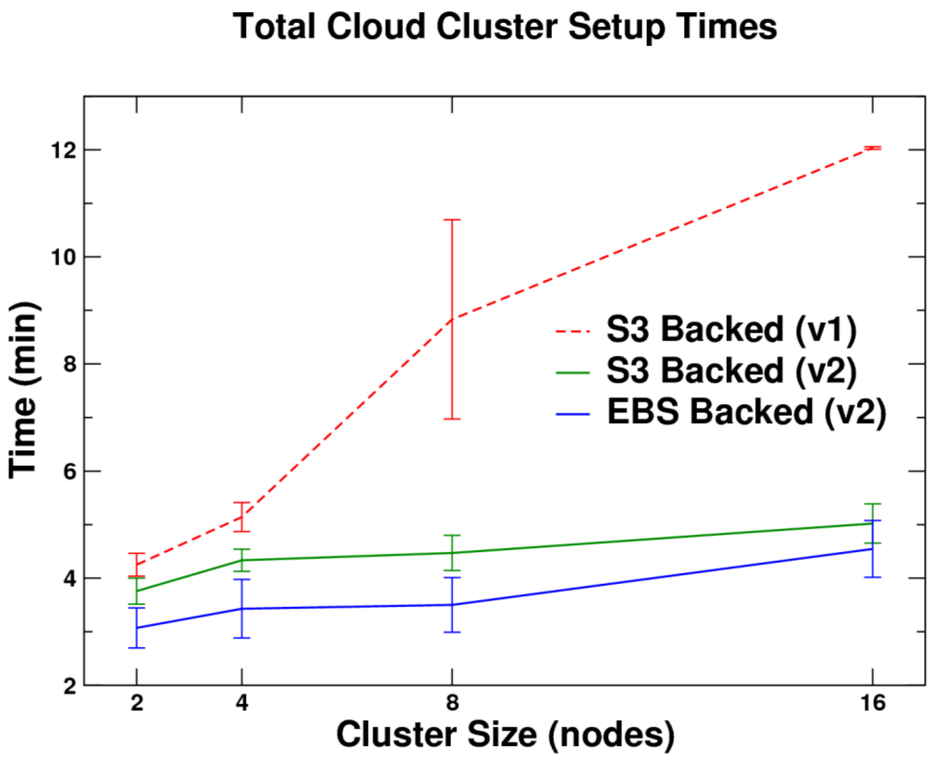
- Older v1 tools :
  - Emphasized simplicity & maximum security
  - SLOW: 12 min for n_{inst}=16, linear with cluster size

- v2 Solutions:
  - Asynchronous tools: minimal setup, max. security
  - Self-Assembling clusters: fast, but sacrifices security
  - Current: Hybrid approach; non-sensitive tasks on cloud keeps credentials safe

UW v2 Tools: Boot and Setup Times

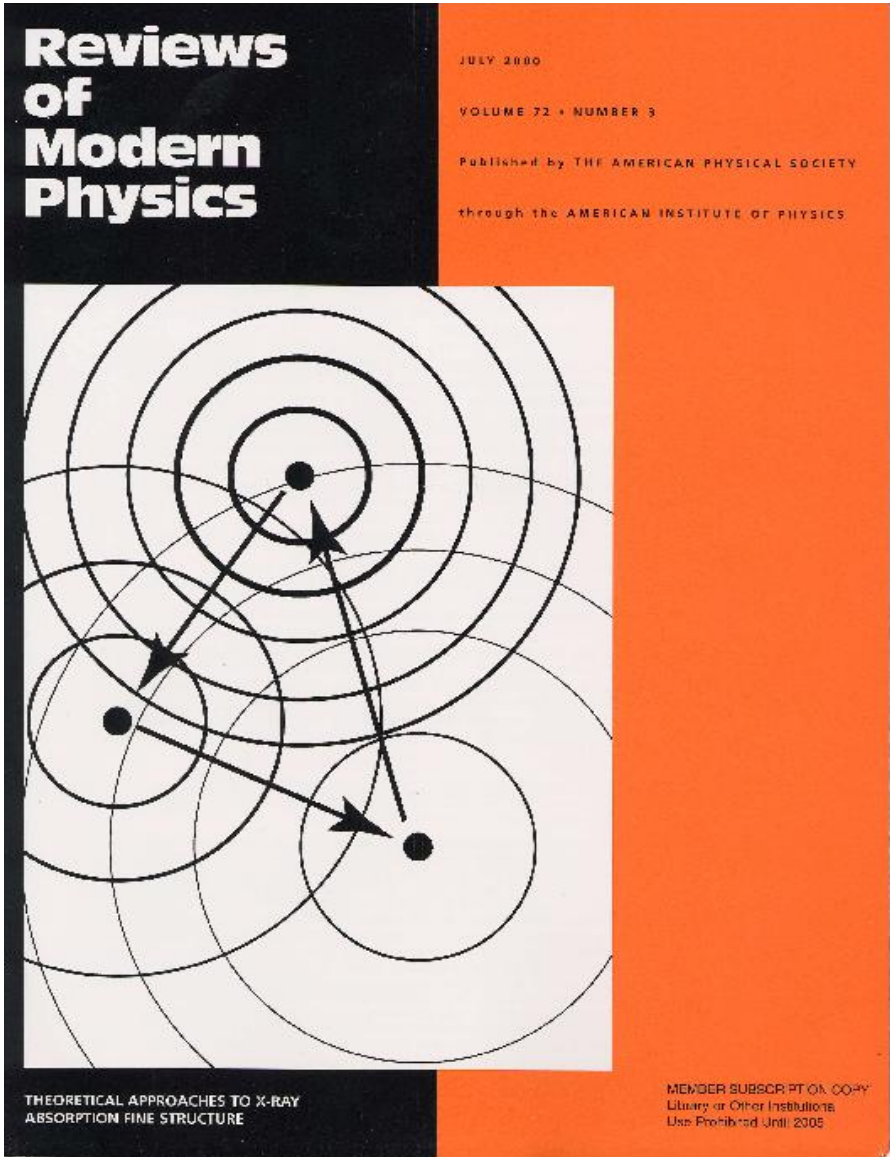

EC2 Boot and Cloud Cluster Setup Times

for S3 Backed Clusters


Total Cloud Cluster Setup Times

- Setup time negligible & independent of cluster size!
- EBS backed clusters faster than S3

Sample Scientific Application



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THEORETICAL APPROACHES TO X-RAY ABSORPTION FINE STRUCTURE

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Use Prohibited Until 2005

FEFF:

Real-space Green’s function code for electronic structure, x-ray spectra, EELS, …

User Base:

1000s of users in physics, chemistry, materials science, biophysics…

J. J. Rehr & R.C. Albers

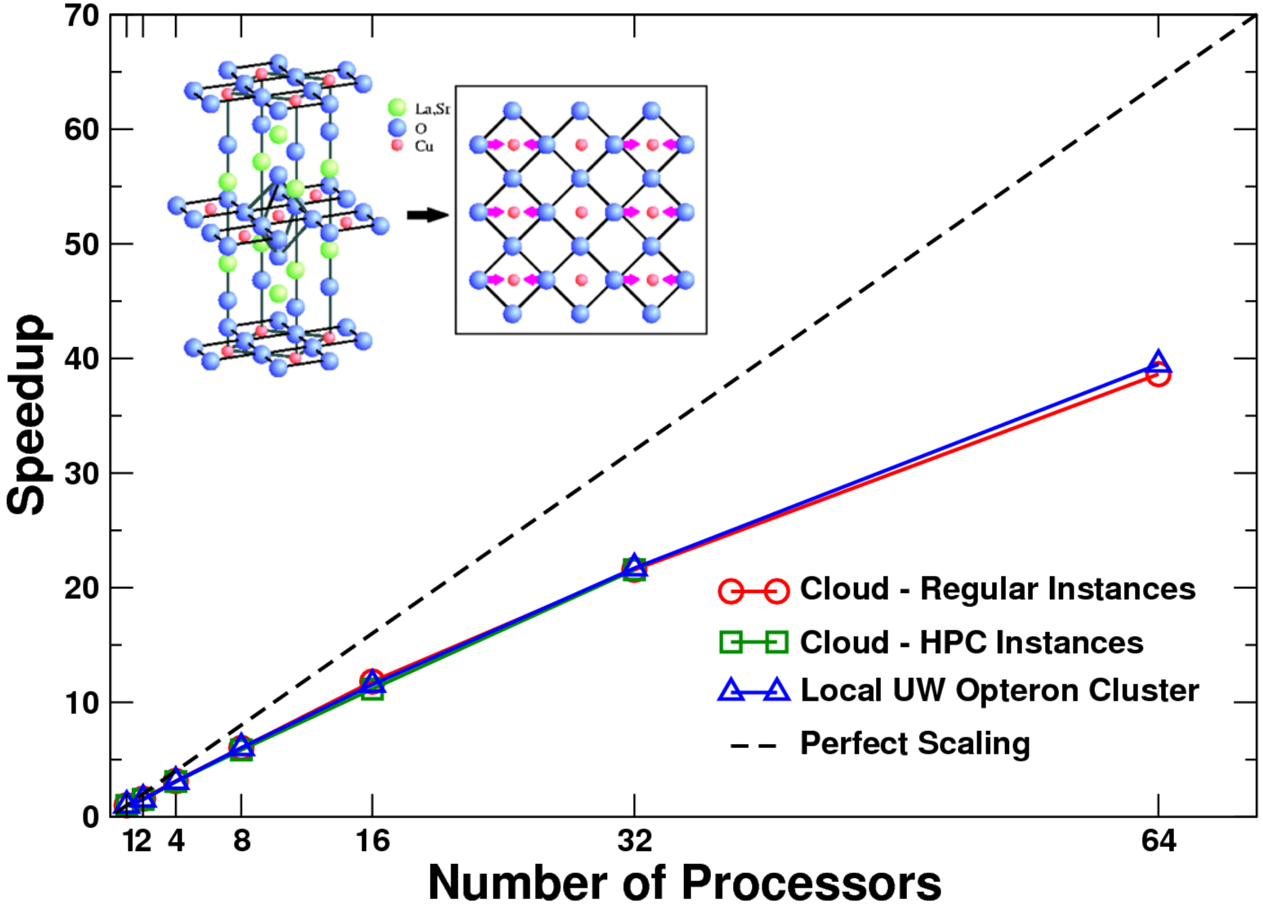
Rev. Mod. Phys. **72**, 621 (2000)

http://leonardo.phys.washington.edu/feff/

FEFF Parallel Performance

Naturally parallel: Each CPU calculates a few points in the energy grid

Loosely coupled: Little communication between processes



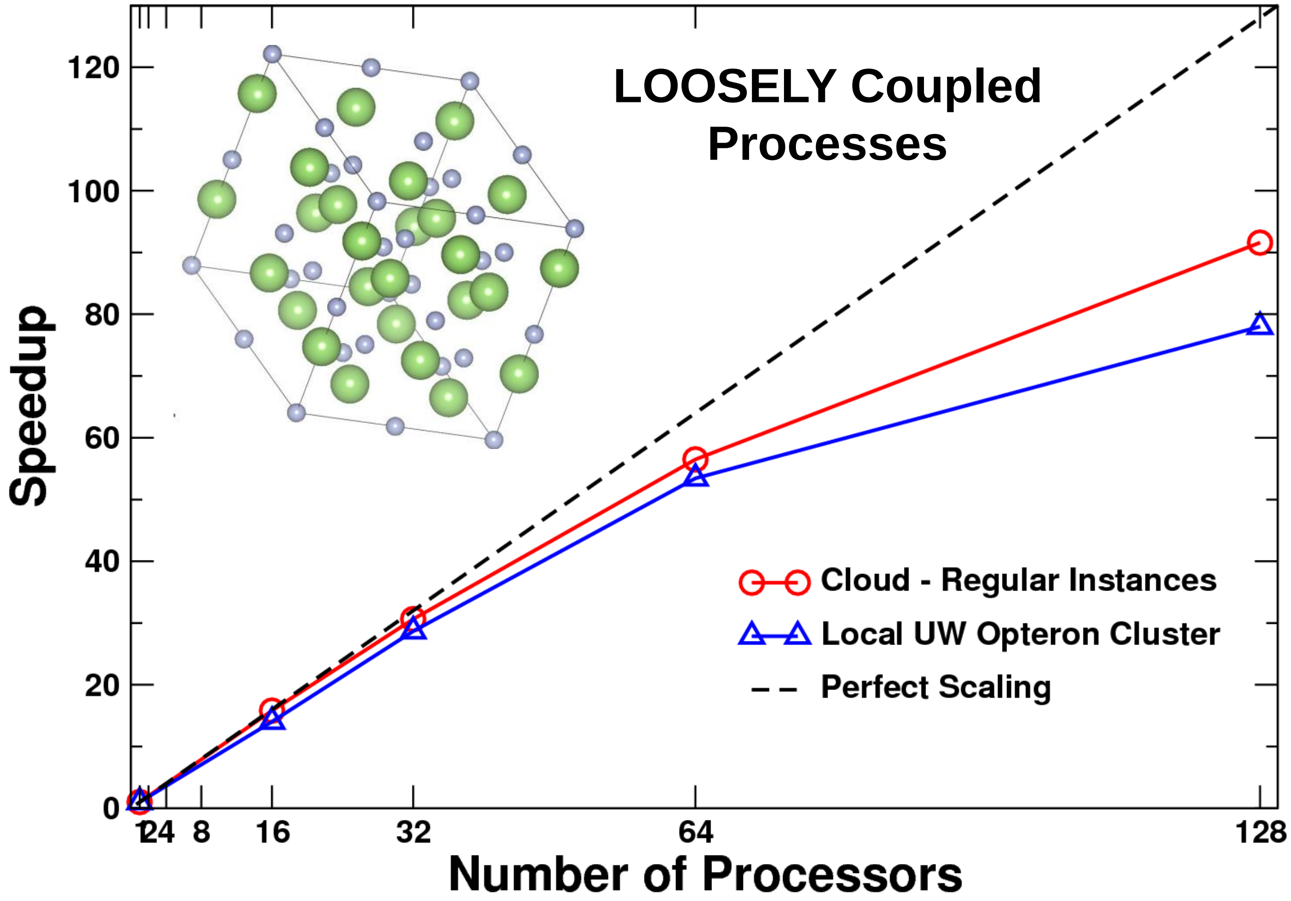
- FEFF9 shows identical speedup on local cluster and EC2 cluster

Sample Electronic Structure Application WIEN2k Parallel Performance

DFT KS equations on
128 k-point grid

Time to solve one
k-point in one core

EC2 small	312s
EC2 medium	116s
EC2 HPC	84s
UW Opteron	189s

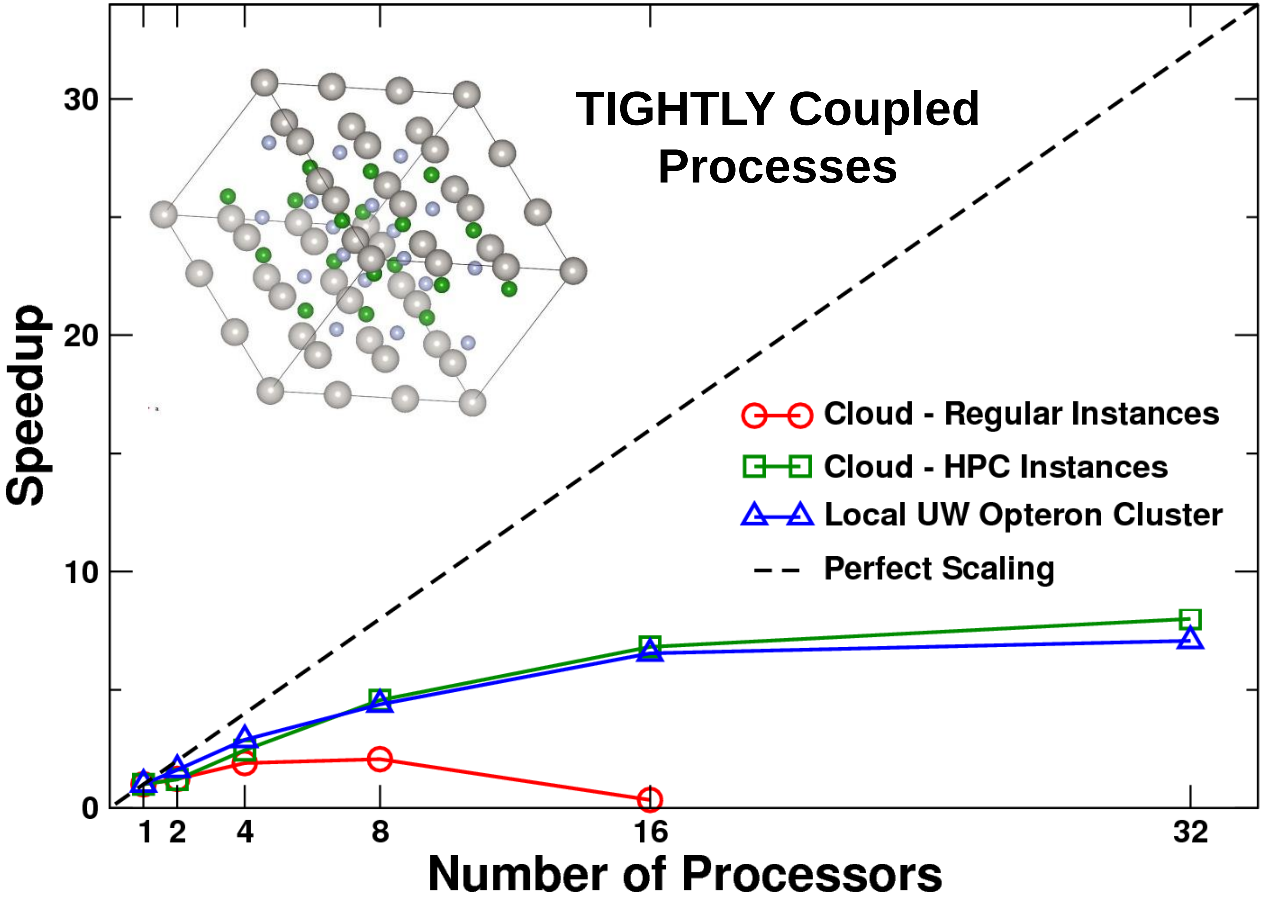


- Good scaling in regular instances

WIEN2k Parallel Performance

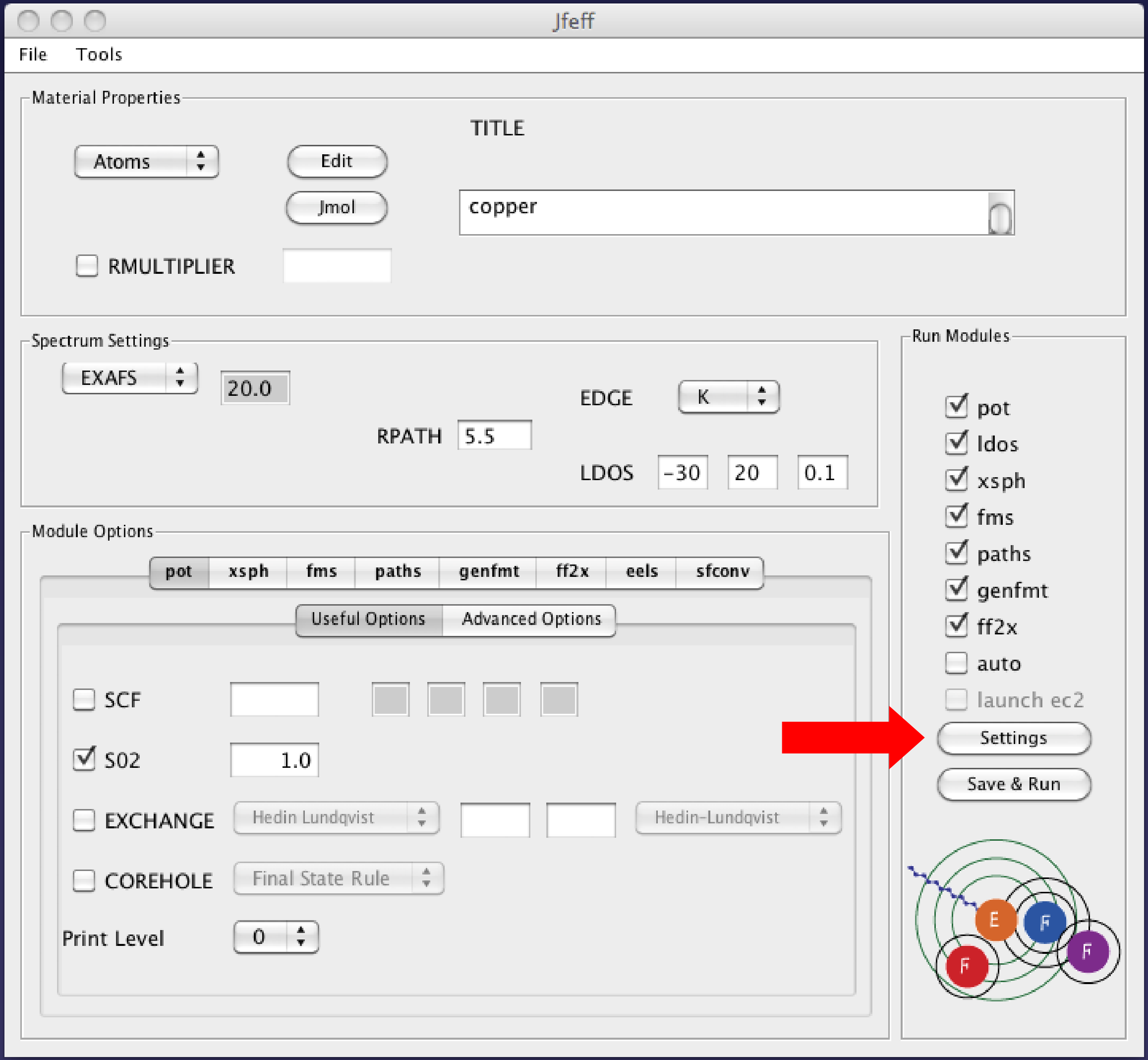
KS for large system at 1 k-point

VERY DEMANDING of network performance



- Regular instances cannot deliver network-intensive performance
- HPC cluster instances deliver the same speedup as local Infiniband cluster

FEFF GUI: XAS on the Cloud



Material Properties

Atoms

TITLE: copper

□ RMULTIPLIER

Spectrum Settings

EXAFS: 20.0

RPATH: 5.5

EDGE: K

LDOS: -30 20 0.1

Module Options

□ SCF

☑ S02: 1.0

□ EXCHANGE: Hedin Lundqvist, Hedin-Lundqvist

□ COREHOLE: Final State Rule

Print Level: 0

Run Modules

☑ pot
☑ ldos
☑ xsph
☑ fms
☑ paths
☑ genfmt
☑ ff2x
□ auto
□ launch ec2

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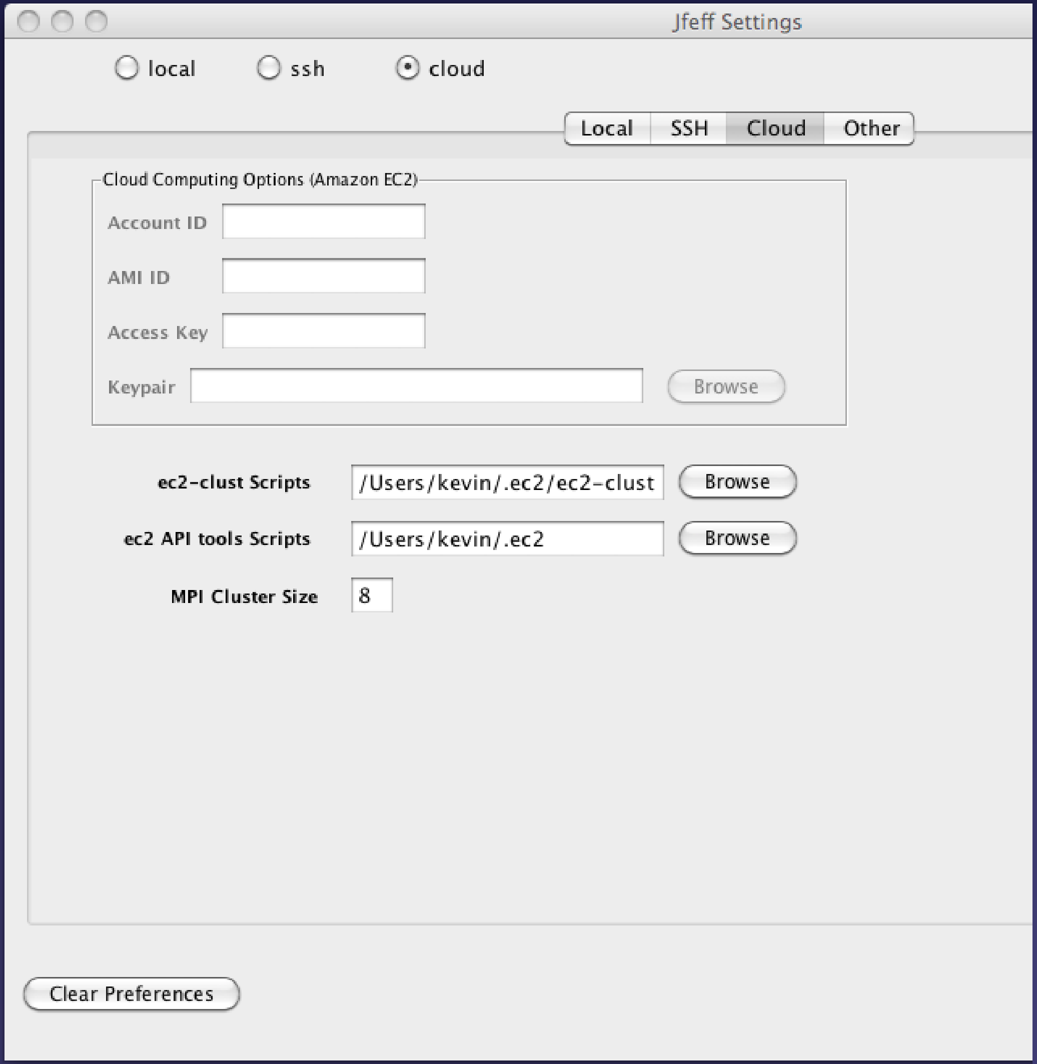


Jfeff Settings

○ local ○ ssh ● cloud

Cloud Computing Options (Amazon EC2)

Account ID

AMI ID

Access Key

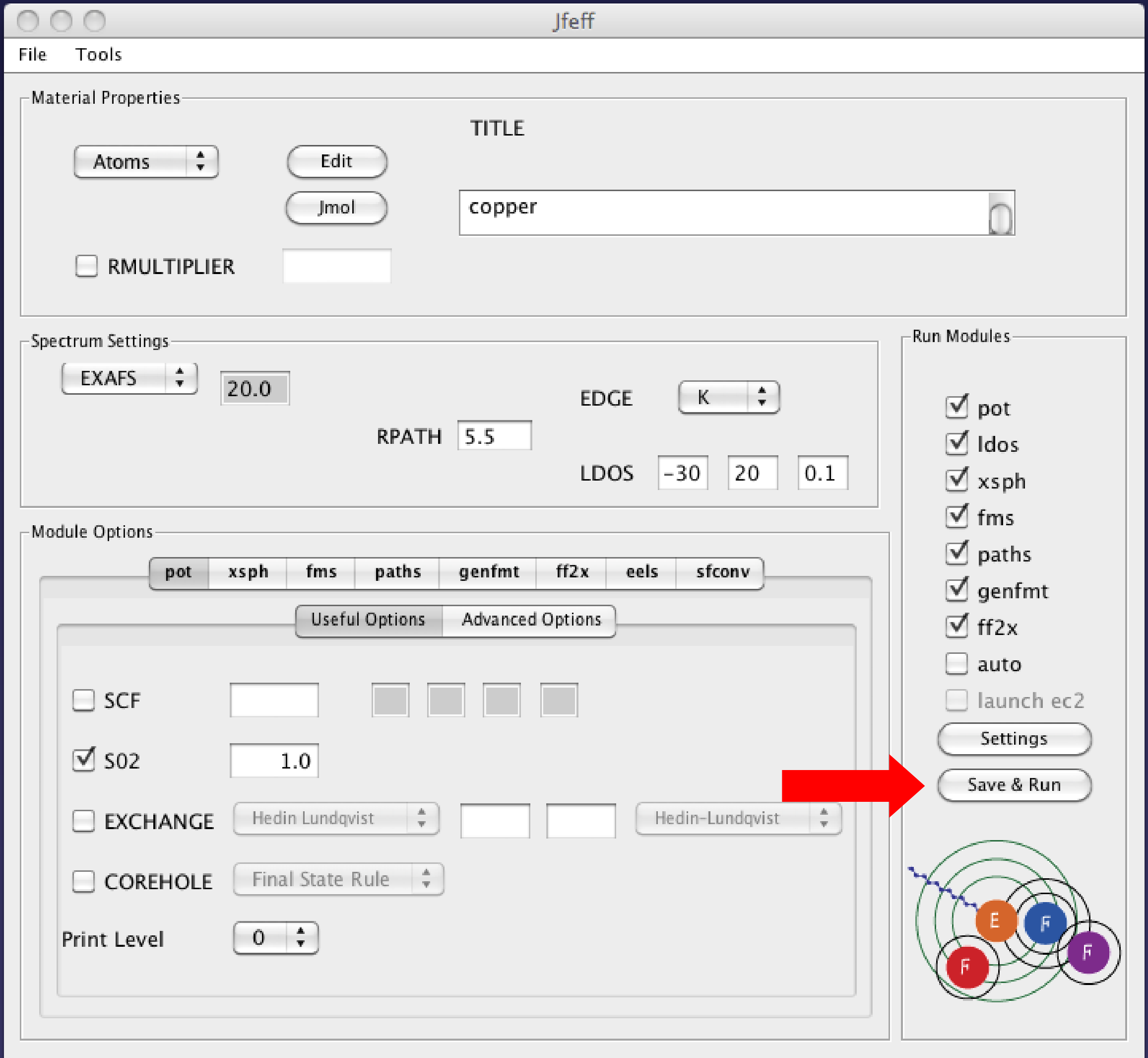
Keypair

ec2-clust Scripts: /Users/kevin/.ec2/ec2-clust

ec2 API tools Scripts: /Users/kevin/.ec2

MPI Cluster Size: 8

FEFF GUI: XAS on the Cloud



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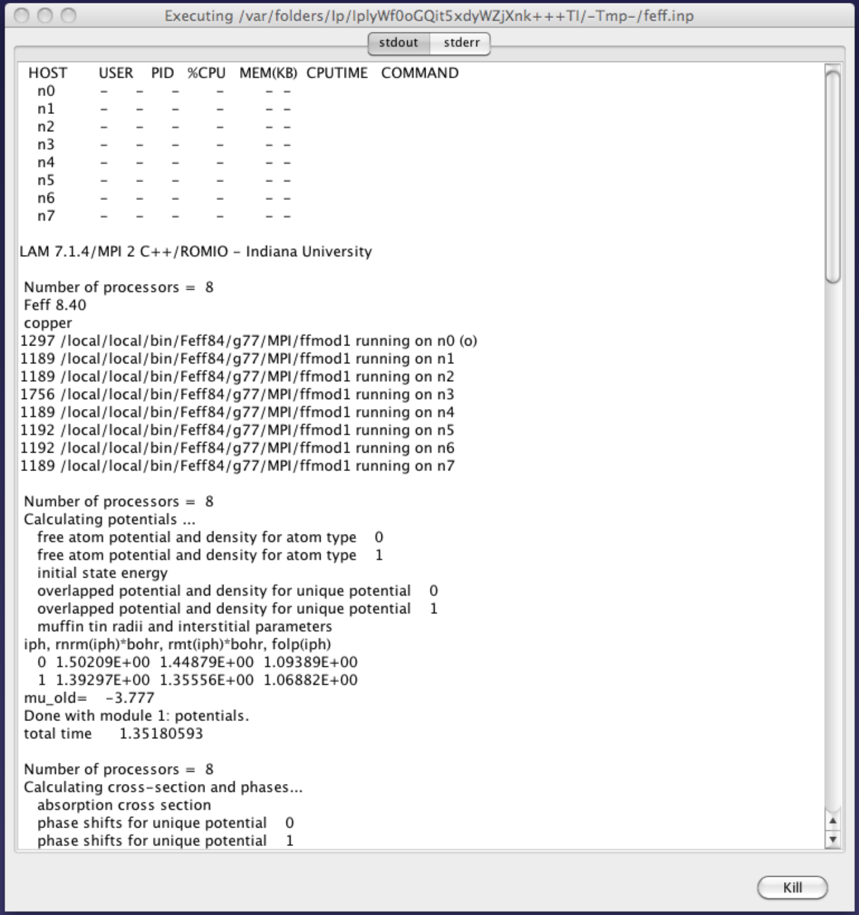
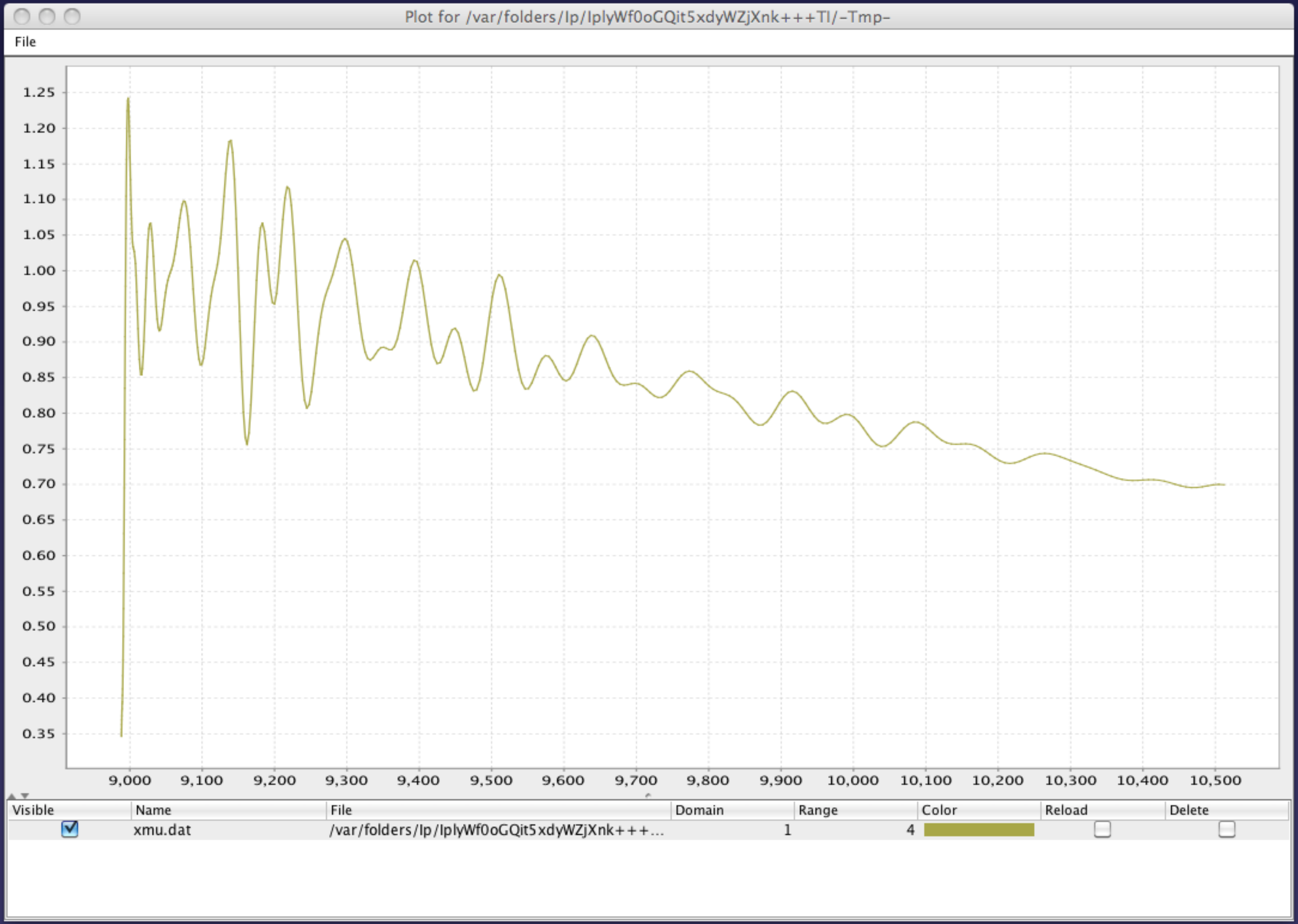


Executing /var/folders/Ip/IplyWf0oGQit5xdyWZjXnk+++TI/-Tmp-/feff.inp
stdout
stderr
Kill

```
 HOST      USER    PID   %CPU    MEM(KB)  CPUTIME   COMMAND
   n0       -     -     -       -       - -
   n1       -     -     -       -       - -
   n2       -     -     -       -       - -
   n3       -     -     -       -       - -
   n4       -     -     -       -       - -
   n5       -     -     -       -       - -
   n6       -     -     -       -       - -
   n7       -     -     -       -       - -

LAM 7.1.4/MPI 2 C++/ROMIO - Indiana University

 Number of processors =  8
 Feff 8.40
 copper
1297 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n0 (o)
1189 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n1
1189 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n2
1756 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n3
1189 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n4
1192 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n5
1192 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n6
1189 /local/local/bin/Feff84/g77/MPI/ffmod1 running on n7

 Number of processors =  8
 Calculating potentials ...
    free atom potential and density for atom type    0
    free atom potential and density for atom type    1
    initial state energy
    overlapped potential and density for unique potential    0
    overlapped potential and density for unique potential    1
    muffin tin radii and interstitial parameters
 iph, rnrm(iph)*bohr, rmt(iph)*bohr, folp(iph)
    0  1.50209E+00  1.44879E+00  1.09389E+00
    1  1.39297E+00  1.35556E+00  1.06882E+00
 mu_old=    -3.777
 Done with module 1: potentials.
 total time       1.35180593

 Number of processors =  8
 Calculating cross-section and phases...
    absorption cross section
    phase shifts for unique potential    0
    phase shifts for unique potential    1
```

FEFF GUI: XAS on the Cloud



Visible	Name	File	Domain	Range	Color	Reload	Delete
☑	xmu.dat	/var/folders/Ip/IplyWf0oGQit5xdyWZjXnk+++...	1	4	🟨	□	□

Conclusions

- Goals partially achieved: robust SCC environment developed & benchmarked on FEFF, WIEN2k
- SCC-ready FEFF App with JFEFF GUI (OSX, Linux)
- Improved SCC AMIs and UW Cluster tools (v2):

  Regular EC2 AMIs OK for light network use

  HPC AMIs NEEDED for MPI+ScaLAPACK

Future Project Goals

- Develop & add WinPC support
- Develop SCC Java GUI for CC management, runs, I/O
- Optimize & benchmark other advanced scientific codes
- Distribute to Scientific Community: http://www.phys.washington.edu/feff/scc

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