Preparation for the Hackathon: Access to Cray KNL System

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ZIB
Outline

- On-line documentation
- Access to HLRN resources
- Ideas for the Hackathon
On-line Documentation Workshop, Cray TDS + HLRN

- [http://tinyurl.com/ZIBCrayTDSDoc](http://tinyurl.com/ZIBCrayTDSDoc)

- Login, uploading a ssh public key
- Access to programs managed by modules (environment)
- (interactive) Batch jobs, KNL mode provisioning
- Using Intel VTune, how to use VNC

- [http://www.hlrn.de](http://www.hlrn.de)
  - HLRN on-line documentation including general TDS topics
Access to HLRN: Upload a Public SSH Key

- Step 1: Generate SSH key pair with passphrase on your local host (laptop)
  ```bash
  localhost$ ssh-keygen
  ```
- Step 2: Login to HLRN Service Portal
  https://zulassung.hlrn.de
- Step 3: Select
  Verwalten Ihrer Keys zum Einloggen auf den HLRN-Rechnern
- Step 4: Login using HLRN username and PIN (see letters)
- Step 5: Select
  Upload eines neuen Schlüssels anfordern
- Step 6: Wait for an email message from HLRN Service Portal with the upload URL
- Step 7: Open URL included in email message
- Step 8: Use „Datei auswählen“ and select the file with the public SSH key for upload
- Step 9: Logout from HLRN Service Portal
- Step 10: Use a SSH client to login in to HLRN
Login to the Cray TDS

- Step 1: login to Berlin HLRN complex
  
  `localhost$ ssh username@blogin.hlrn.de`

  Last login: Mon Sep 26 08:00:00 2016 from ...
  
  `blogin1:~ $`

- Step 2: login to bxcmomtds1 (MOM and interactive working node)
  
  `blogin1:~ $ ssh bxcmomtds1`

  Last login: Mon Sep 26 08:02:00 2016 from ...
  
How to Access the Intel Parallel Studio XE

- Switch to Intel Programming Environment

```
bxcmomtds1:~> module switch PrgEnv-cray PrgEnv-intel
bxcmomtds1:~> ftn -V
```

Intel(R) Fortran Intel(R) 64 Compiler for applications running on Intel(R) 64, Version 17.0.0.098 Build 20160721
Copyright (C) 1985-2016 Intel Corporation. All rights reserved.
Loading a Cray Developer Toolkit

- Load a Cray Developer Toolkit (CDT)
  
bxcmomtds1:~> module load cdt
  Switching to atp/2.0.2.
  Switching to cce/8.5.3.
  Switching to cray-libsci/16.09.1.
  Switching to cray-mpich/7.4.3.
  Switching to craype/2.5.7.
  Switching to modules/3.2.10.5.
  Switching to pmi/5.0.10-1.0000.11050.0.0.ari.
  bxcmomtds1:~>
Prepare for Using the Cray Performance Analysis Tools

- Step 1: load the Cray Developer Toolkit
  bxcmomtds1:~> module load cdt

- Step 1: load the Cray Performance Analysis Tools
  bxcmomtds1:~> module load perftools-base
  bxcmomtds1:~> module load perftools[-lite]
  bxcmomtds1:~> pat_build -V
  CrayPat/X: Version 6.4.1 Revision 6a6694f 06/27/16 17:24:11
Ideas for the Hackathon
“Lab Book”: Keep the Records of Your Work

- Make a note of the initial performance for future reference.
  - May use different compilers (Intel, Cray, GCC)

- Make notes both of your optimization steps and the achieved performance.
  - This is valuable information for you and for us!

- Prepare a summary of the achieved results
  - Present it on Day 3 morning, and optionally send to steinke@zib.de
  - We like to learn about best-practice solutions and what failed
Organization of Work

- Define your environment ...
  - ... to build your application
  - ... to run your application
  - Make lab book notes

- Hackathon teams ... (same code, same research group)