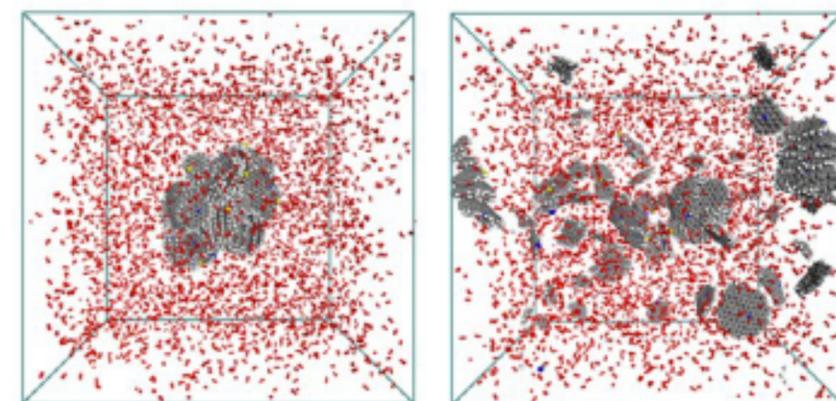
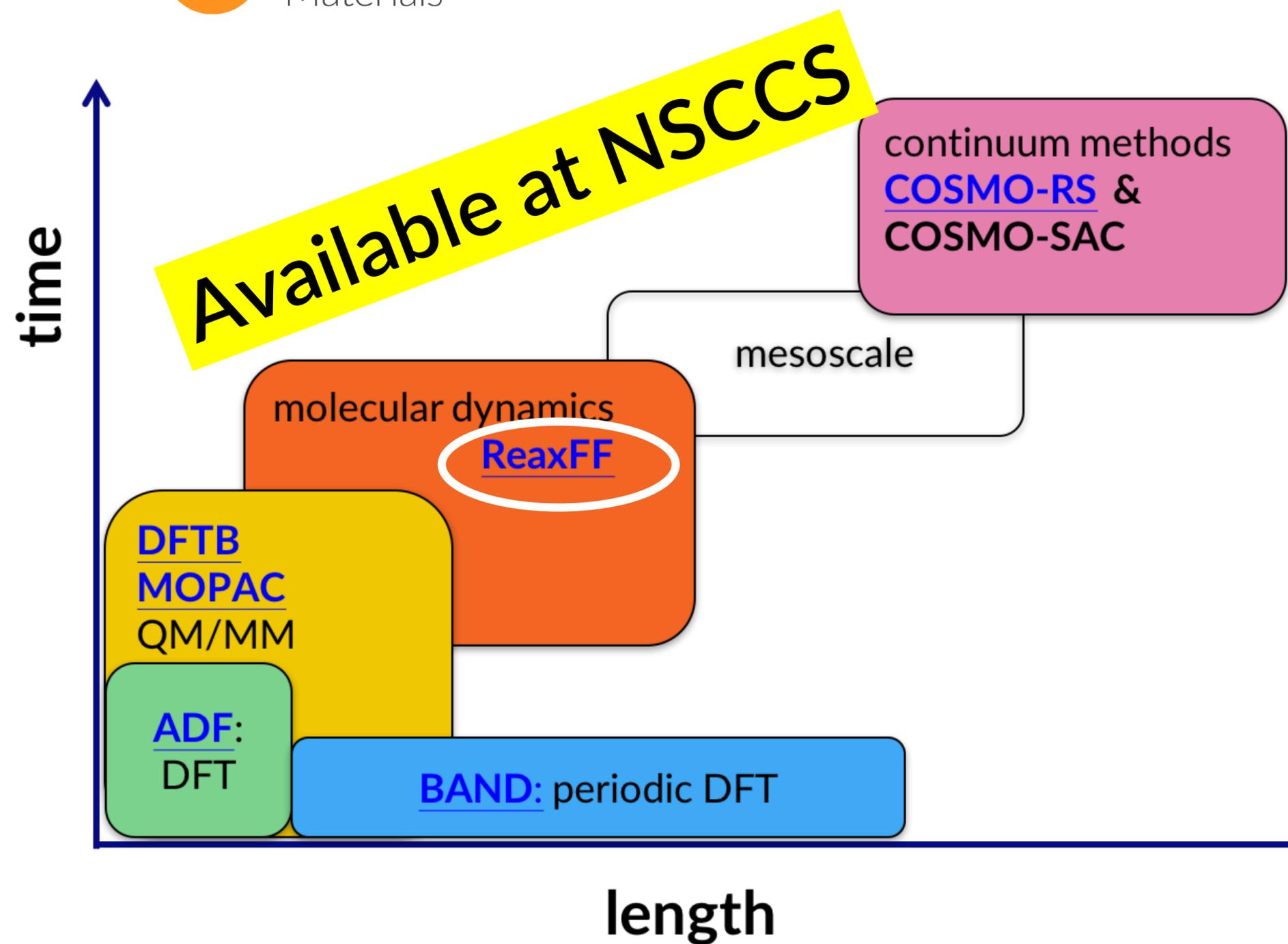
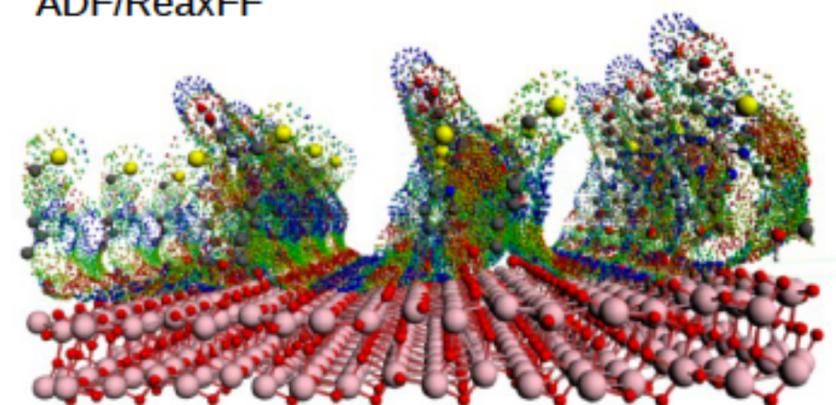


& the ADF Modeling Suite



ADF/ReaxFF



BAND



ADF

NSCCS 27-28 September 2016

Ole Carstensen – carstensen@scm.com
Fedor Goumans – goumans@scm.com
Anna Shchygol – shchygol@scm.com

Workshop program (changed)

Day 1:

11.15-12.00: Intro to ADF & ReaxFF

Getting started with the GUI

Running ADF from the command line in Windows

13.00-14.00: **force bias Monte Carlo**: introduction & hands-on healing graphene

15.15-17:30: Intro to GCMC

hands-on: choose from **GCMC** or **ChemTraYzer**

hands-on: analyzing fbMC results with python (while GCMC or combustion is running)

Day 2:

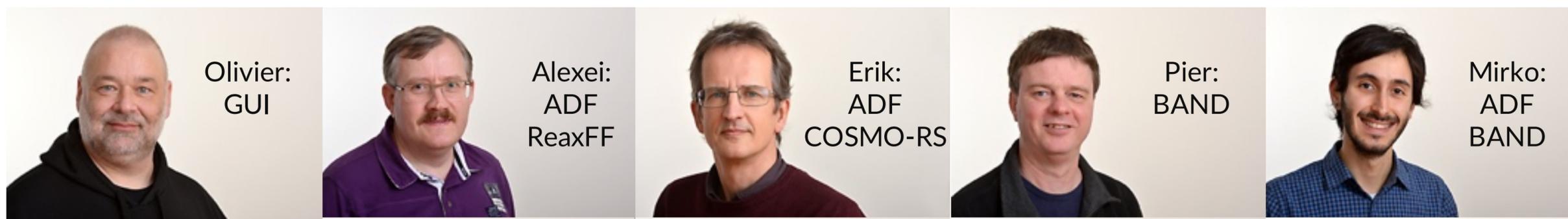
11:00-12.00: Demo + hands-on: **building a ReaxFF force field**: how to get started with reasonable guesses?

13:00-15:00: Hands-on: **building a training set** + optimizing a ReaxFF with **MCFF**

15:30-16.15: Wrap up previous tutorials / individual questions problems

The SCM team

Developers



Business



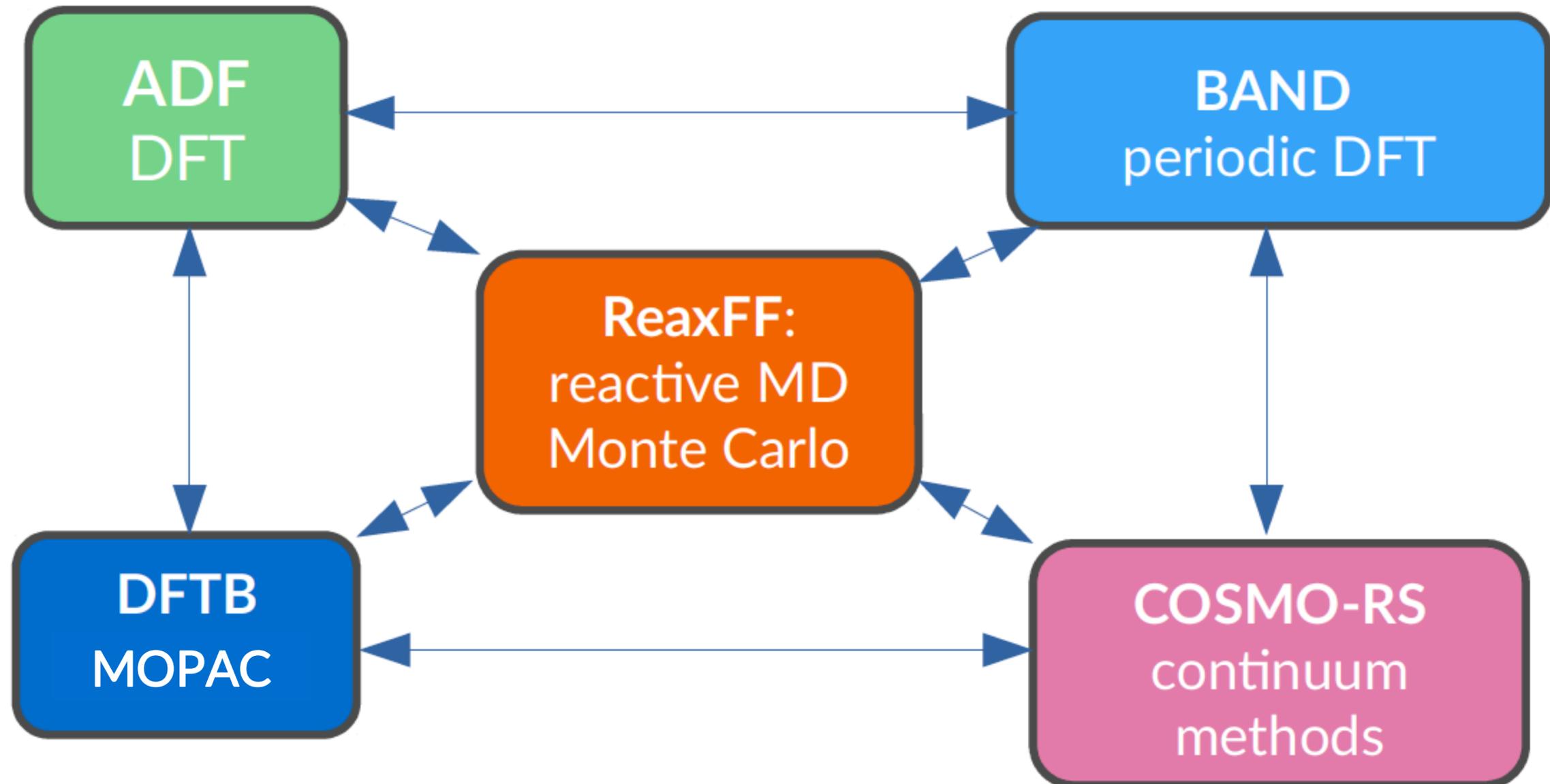
EU fellows



+ many academic collaborations interested? lopez@scm.com

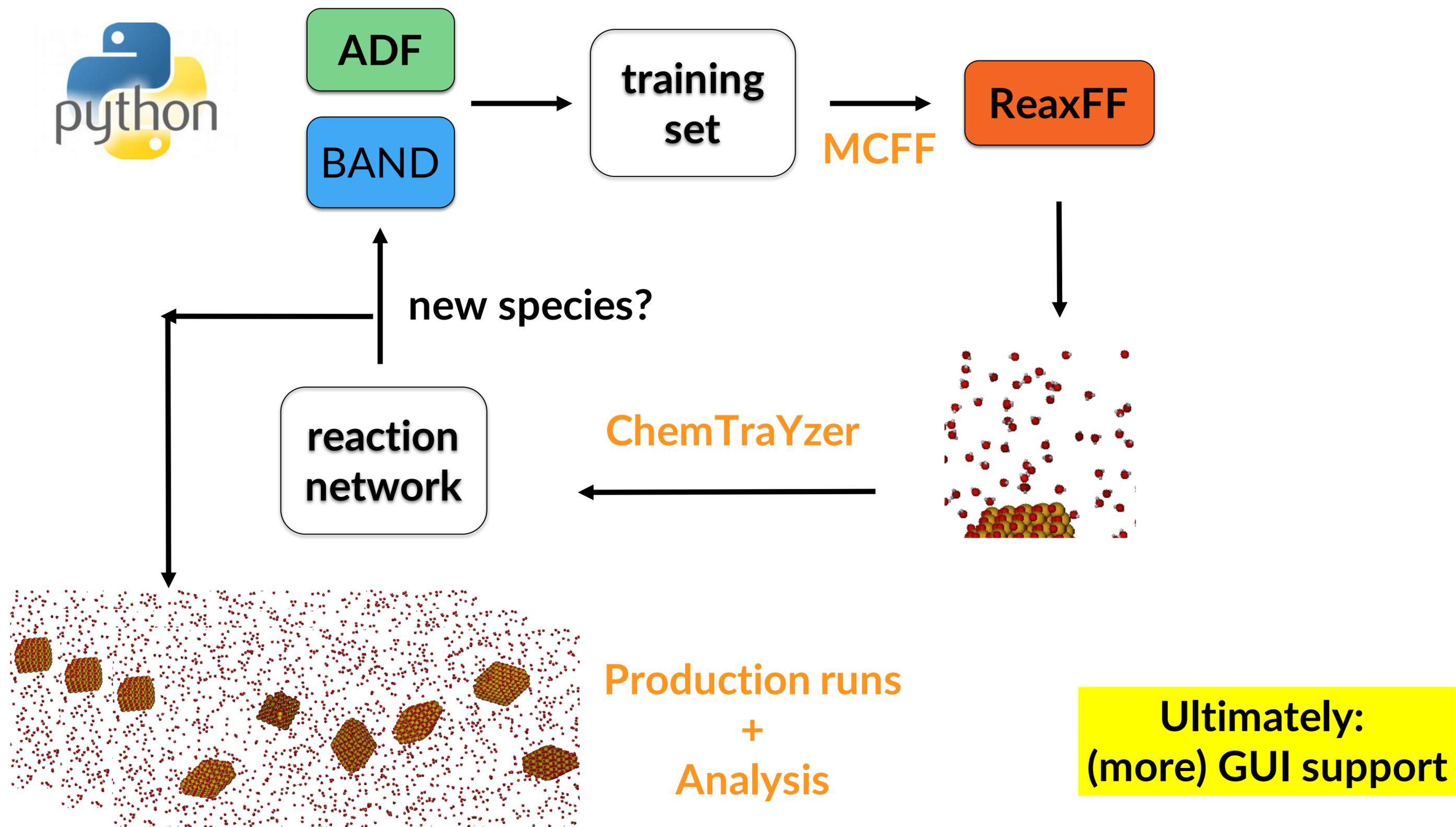


Tying it all together: python



Links all modules + various tools
→ workflows & screening
→ (custom) post-processing
→ rapid prototyping

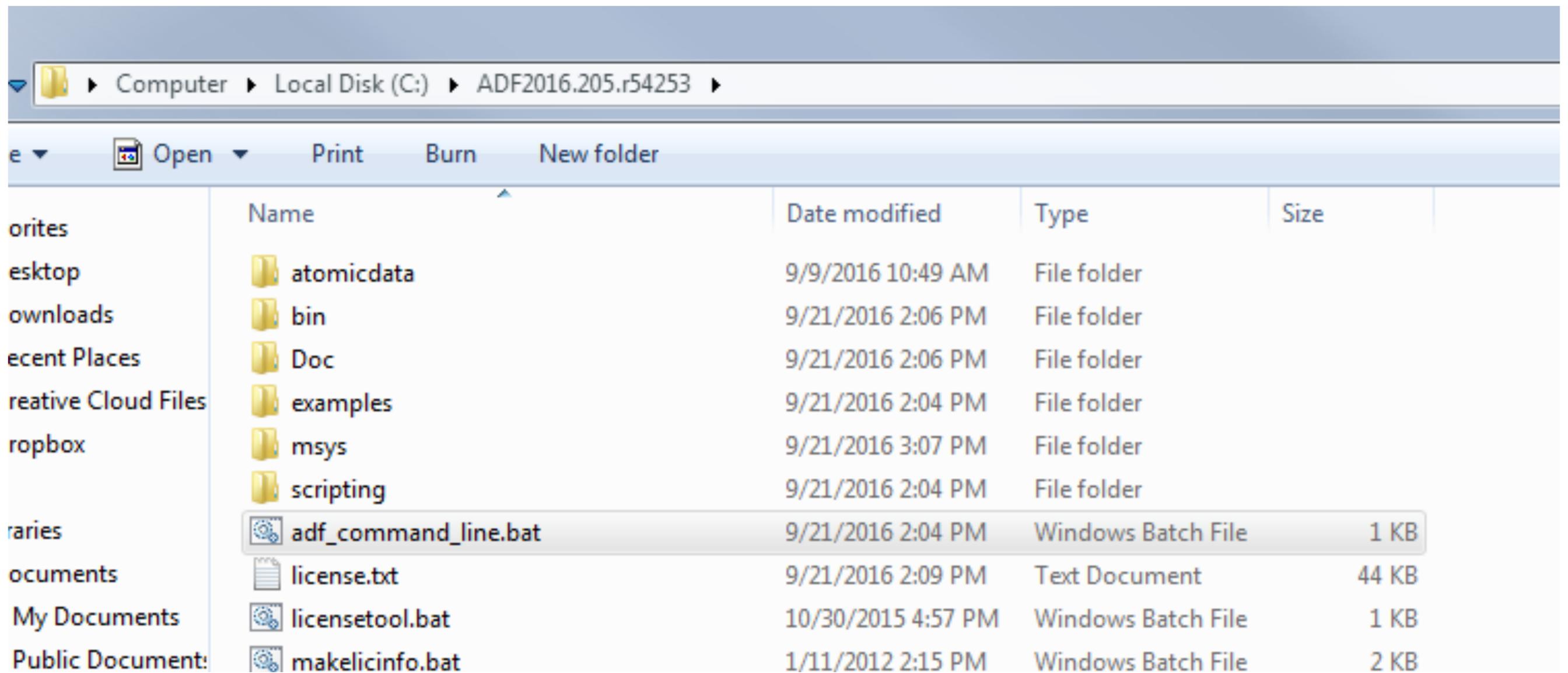
Automating ReaxFF parameterization



Scripting on Windows

In Windows install dir: double click `adf_command_line.bat`

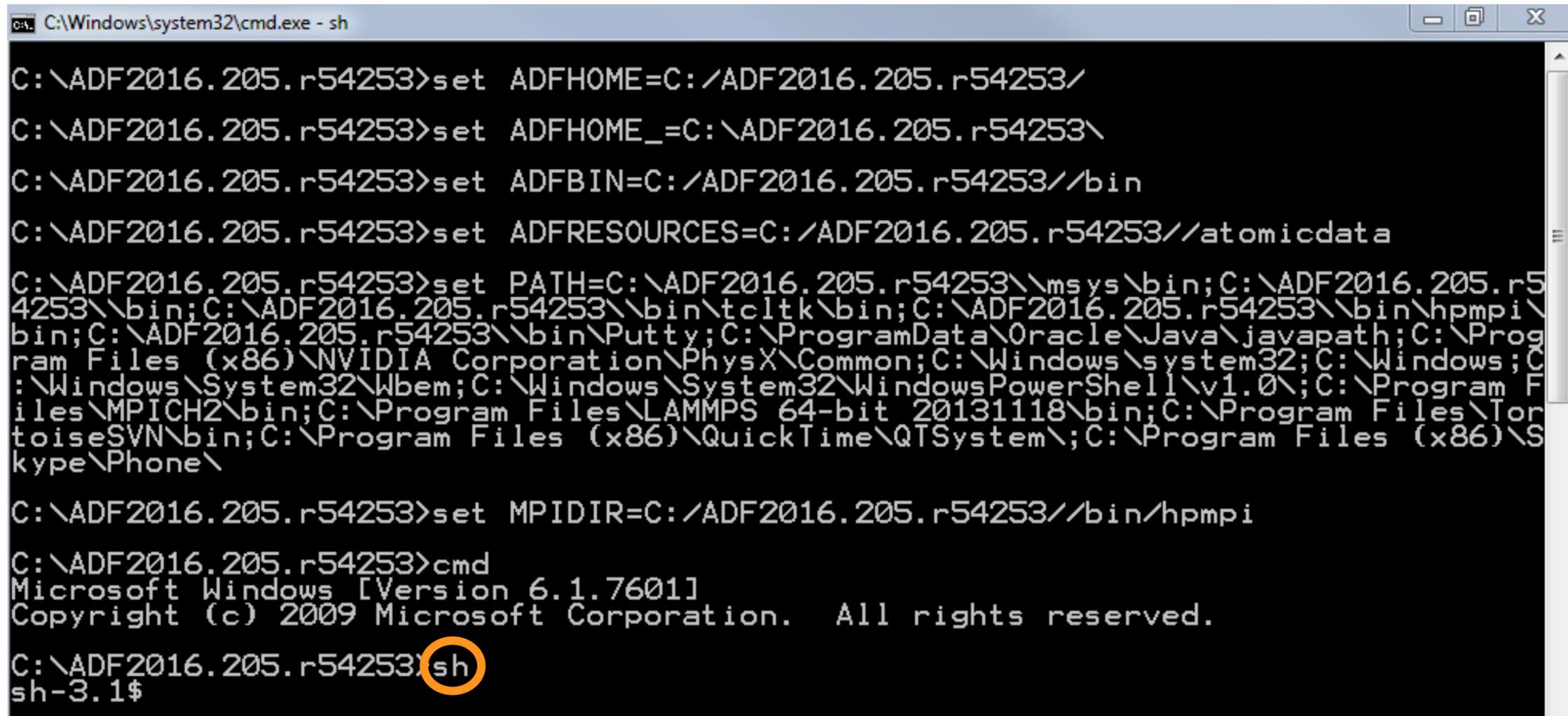
This will open a cmd shell with all variables set



Scripting on Windows

Shell commands can now be run, including ADF

To get even more shell-like: issue `sh` in the cmd prompt



```
C:\Windows\system32\cmd.exe - sh
C:\ADF2016.205.r54253>set ADFHOME=C:/ADF2016.205.r54253/
C:\ADF2016.205.r54253>set ADFHOME_=C:\ADF2016.205.r54253\
C:\ADF2016.205.r54253>set ADFBIN=C:/ADF2016.205.r54253/bin
C:\ADF2016.205.r54253>set ADFRESOURCES=C:/ADF2016.205.r54253/atomicdata
C:\ADF2016.205.r54253>set PATH=C:\ADF2016.205.r54253\msys\bin;C:\ADF2016.205.r54253\bin;C:\ADF2016.205.r54253\bin\tcltk\bin;C:\ADF2016.205.r54253\bin\hpmpi\bin;C:\ADF2016.205.r54253\bin\Putty;C:\ProgramData\Oracle\Java\javapath;C:\Program Files (x86)\NVIDIA Corporation\PhysX\Common;C:\Windows\system32;C:\Windows;C:\Windows\System32\Wbem;C:\Windows\System32\WindowsPowerShell\v1.0;C:\Program Files\MPICH2\bin;C:\Program Files\LAMMPS 64-bit 20131118\bin;C:\Program Files\TorsoiseSVN\bin;C:\Program Files (x86)\QuickTime\QTSystem\;C:\Program Files (x86)\Skype\Phone\
C:\ADF2016.205.r54253>set MPIDIR=C:/ADF2016.205.r54253/bin/hpmpi
C:\ADF2016.205.r54253>cmd
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.
C:\ADF2016.205.r54253>sh
sh-3.1$
```

Not as powerful as *nix shell

Windows may have file permissions issues: opening/editing files 'in use'

Be aware of conversions issues (^M in scripts made on Windows)

Python Scripting on Windows

Use startpython to use the python stack shipped with ADF
To access plams + python scripts used during this workshop

```
sh-3.1$ startpython get_defects.py ReaxFF_London_fbMC.rxkf
[15:37:56] PLAMS working folder: c:\ADF_DATA\plams.460
0          20
50         22
100        20
150        19
200        17
250        17
300        18
350        18
400        19
450        17
500        16
550        14
600        12
650        12
700        12
750        12
800        10
850        10
900        10
950        10
1000       10
sh-3.1$
```

Questions? Problems?: support@scm.com or adf mailing list