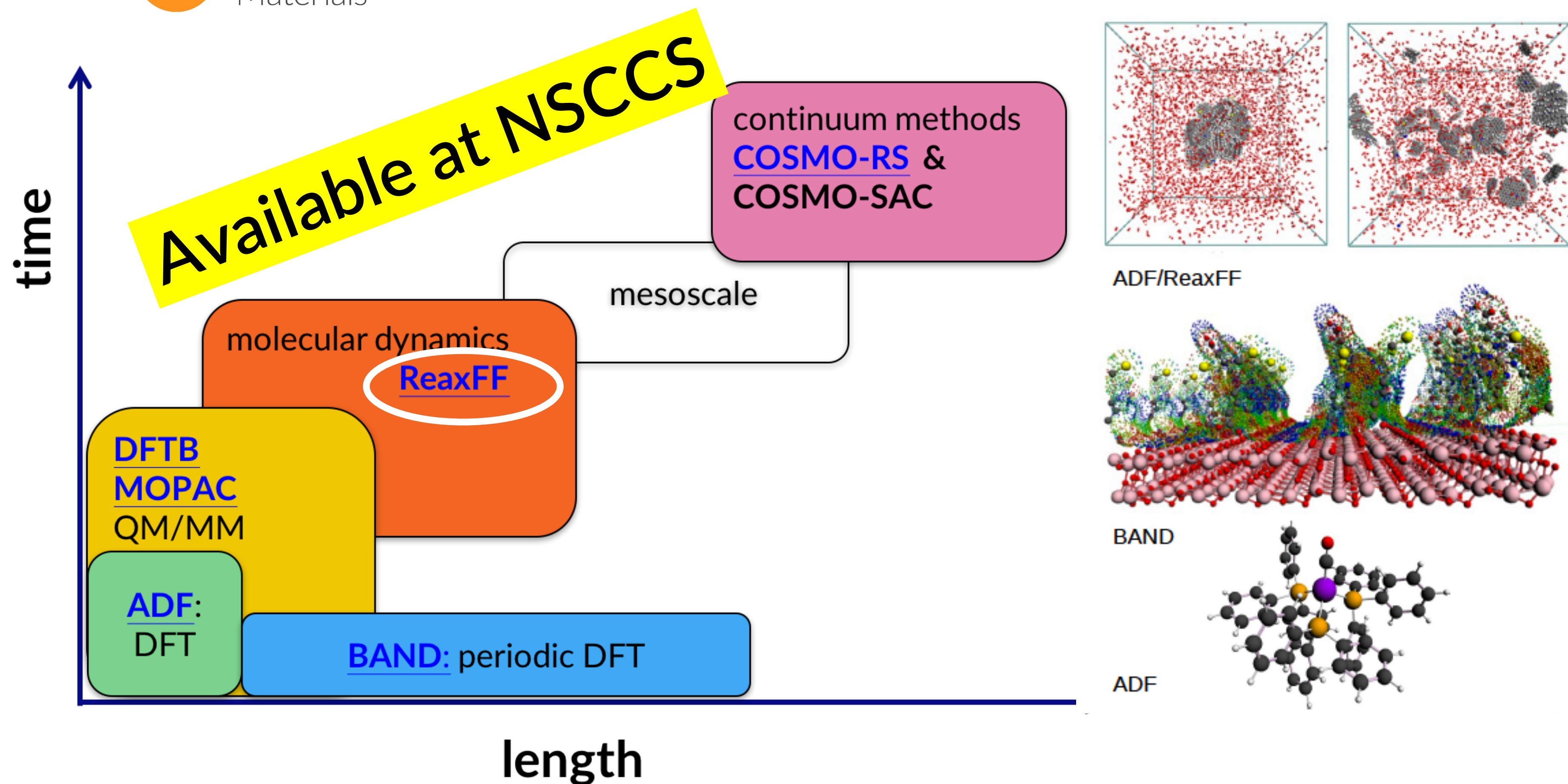


& the ADF Modeling Suite



NSCCS 27-28 September 2016

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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

	Olivier: GUI		Alexei: ADF ReaxFF		Erik: ADF COSMO-RS		Pier: BAND		Mirko: ADF BAND
	Hans: Linux GPU Python		Thomas: DFTB Scripting		Laurens: GUI		Ole: GUI ReaxFF		Evert Jan: Adviser
	Stan: CEO		Fedor: Marketing		Sergio: Collaborations		Frieda: Invoices Licenses		Kitty: Finance
	Marc: BAND		Damien: Scripting MOFs		Anna: ReaxFF MOFs		Michal, Robert: QM/MM, excited states MD		
									

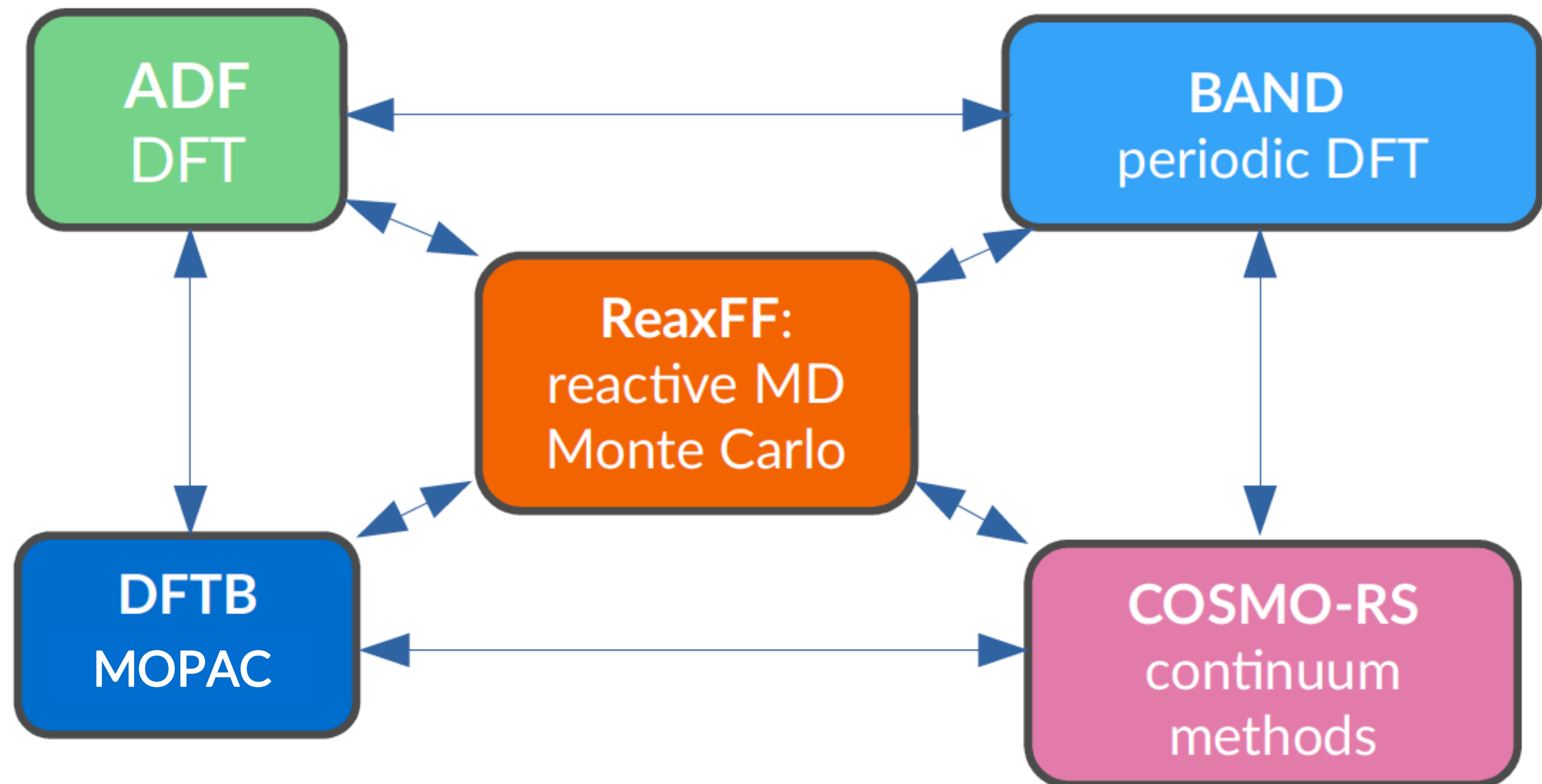
EU fellows

Business

+ many academic collaborations
interested? lopez@scm.com

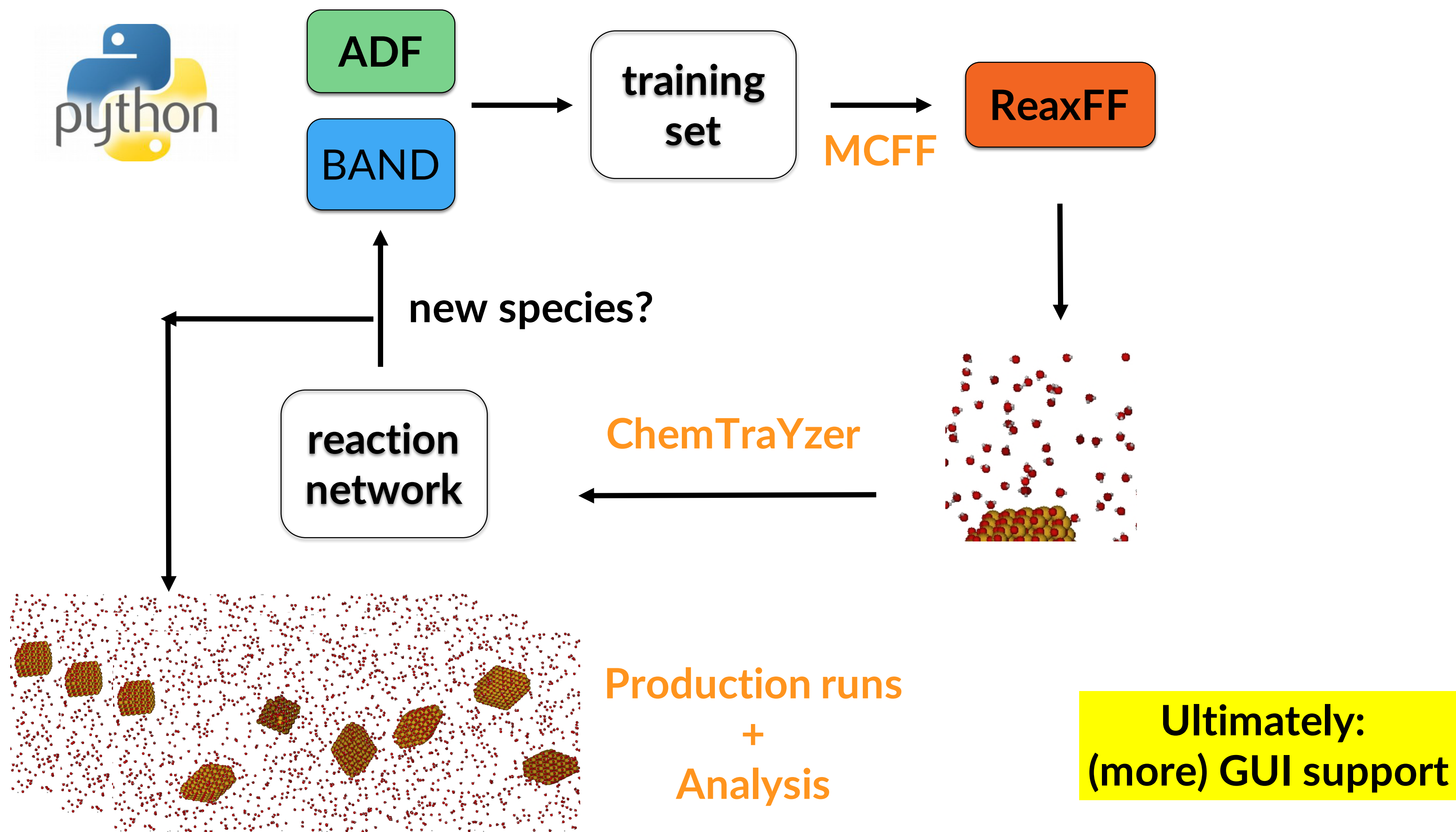


Tying it all together: python



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

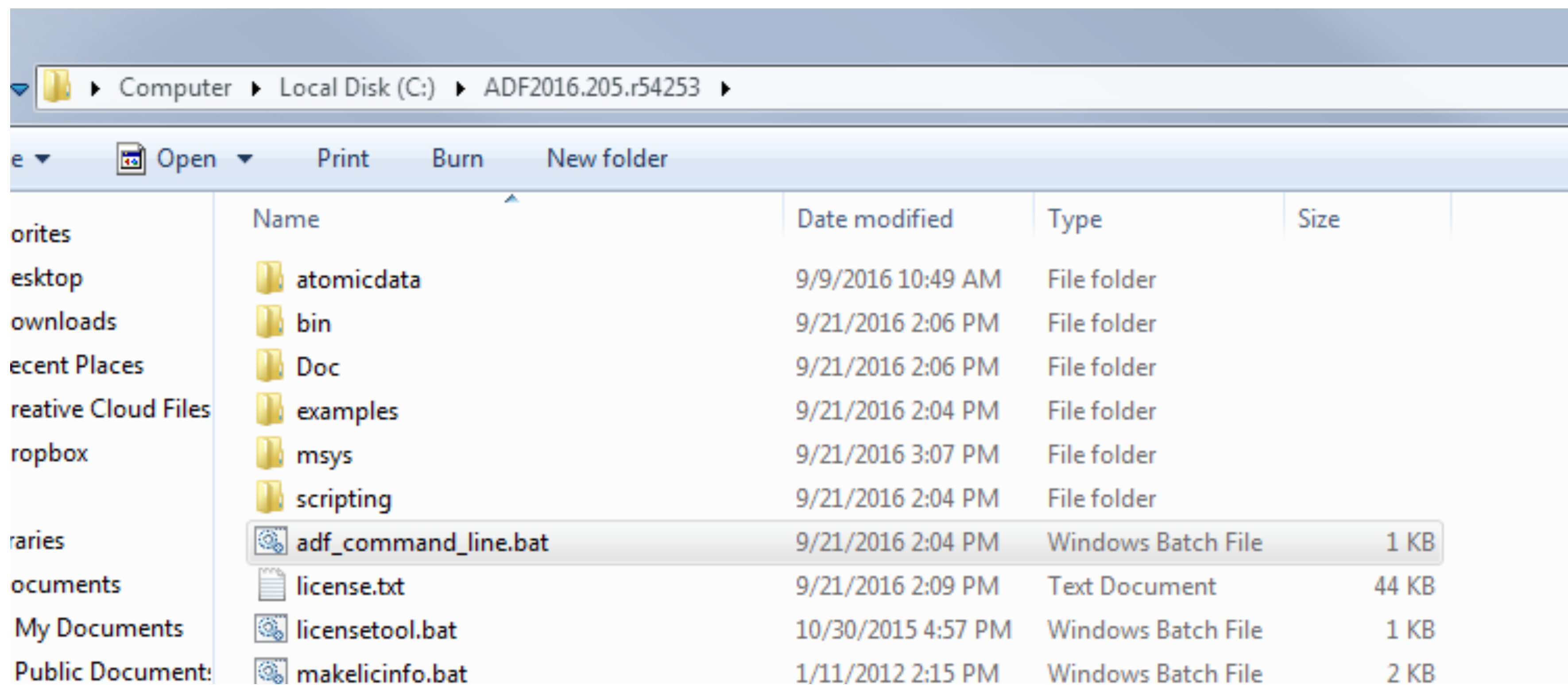
Automating ReaxFF parameterization



Scripting on Windows

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

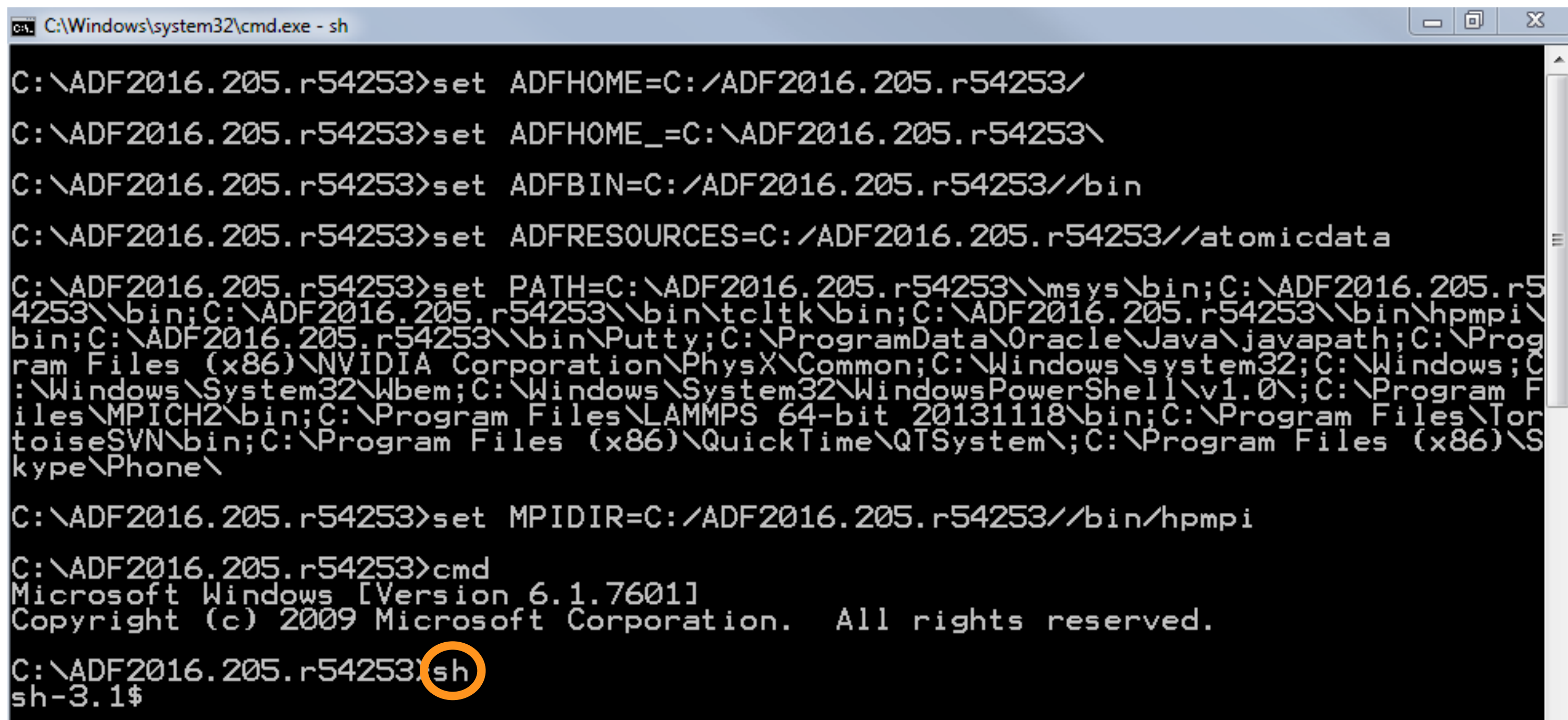
This will open a cmd shell with all variables set



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\hpmi\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)\Sony\Phone\
C:\ADF2016.205.r54253>set MPIDIR=C:/ADF2016.205.r54253/bin/hpmi
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