Introduction

The "build" script

The End 0000000000

A universal OpenFOAM build script Using Ansible to make your machine "OpenFOAM ready"

Bernhard F.W. Gschaider

HFD Research GesmbH

Graz 3. July 2019

Heinemann Fluid Dynamics Research GmbH

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Graz 3. July 2019 1 / 53

Introduction • • • • • • • • • • • • • • • • • • •	Ansible 000000000000000000000000000000000000	The "build" script
Outline		
 Introduction This presenta Who is this? What is your Ansible What it is 	problem?	 Advanced Ansible The "build" script Preparation Building Supported The End Controversial top
How it works		Goodbye

The End

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Introduction	Ansible 00000000000000000	The "build" script
This presentation		
Outline		
 Introduction This presen Who is this What is you Ansible What it is 	? Ir problem?	 Advanced Ansible The "build" script Preparation Building Supported The End Controversial topics
How it work	(5	Goodbye

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Graz, 2019-07-03 3 / 53

The End

 The "build" script

The End

What it's about

A programmer is a person that does a lot of work because he is lazy

I often compile OpenFOAM

And sometimes I have to set up machines to do so

- This is repetitive work
- So I wrote something to do it for me
- In the time I could have set up a lot of machines
 - To make it worth the while other people should use it

Introductio	0000	Ansible 00000000000000	The "build" script 00000000000000000000	The End
Outli				
1	Introduction This presentation Who is this? What is your provided the second		 Advanced Ansible The "build" script Preparation Building Supported 	
2	Ansible What it is How it works		 4 The End Controversial topics Goodbye 	

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Graz, 2019-07-03 5 / 53 Introduction OCOBOOOOOO Who is this? The "build" script

The End

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- Working with OPENFOAM[™] since it was released
 - Still have to look up things in Doxygen
- I am not a core developer
 - But I don't consider myself to be an *Enthusiast*
- My involvement in the OPENFOAM[™]-community
 - Janitor of the openfoamwiki.net
 - Author of two additions for OPENFOAM[™]

swak4foam Toolbox to avoid the need for C++-programming

PyFoam Python-library to manipulate OPENFOAM[™] cases and assist in executing them

■ Organizing committee for the OPENFOAM[™] Workshop

• The community-activies are not my main work but *collateral damage* from my real work at ...

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Introduction 0000000000 Who is this? The "build" script

The End 0000000000

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Description

- Located in Leoben, Austria
 - ... and Vienna
- Works on
 - Fluid simulations
 - OPENFOAM[™] and Closed Source
 - Software development for CFD
 - mainly OPENFOAM[™]
- Industries we worked for
 - Automotive
 - Processing

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Introduction	Ansible 000000000000000000000000000000000000	The "build" script
What is your problem?		
Outline		
 Introduction This presentat Who is this? What is your Ansible What it is How it works 		 Advanced Ansible The "build" script Preparation Building Supported The End Controversial topics Goodbye

The End

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Graz, 2019-07-03 8 / 53

Introduction OCOCO What is your problem? The "build" script

The End 0000000000

Binary distributions

There are OpenFOAM-binaries

- The Foundation supplies Ubuntu-Packages
- OpenCFD supplies RPM-packages
- Both supply Docker-images that run on Linux, Windows and MacOS
- There is a number of binaries rolled by other people



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Introduction 0000000000 What is your problem? The "build" script

The End 0000000000

Why I still compile OpenFOAM

- Docker makes me uneasy
 - Especially if people don't publish their Dockerfile
- There is no binary for this OpenFOAM version on this operating system
- I often need a Debug-version
 - Because my code has bugs
- Sometimes I need an ancient version of OpenFOAM
 - Recently compiled OpenFOAM 2.3. Don't ask

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Graz, 2019-07-03 10 / 53

Introduction OCOCOCOO What is your problem? The "build" script

The End

Steps to compile

Compilation always requires similar steps

- 1 Make sure the required software is installed
- 2 Get the sources
- 3 Put the sources in the right place
- 4 Download the necessary third-party sources
- 5 Extract in the correct places
- 6 Edit configuration to use the correct versions
- 7 Start the compilation
- 8 Curse because I forgot one of steps 1-6
- It is not rocket science but repetitive error-prone work
 - which is the worst kind of work

Introduction OCOCOCOO What is your problem? The "build" script

The End

Bonus: compile the compiler

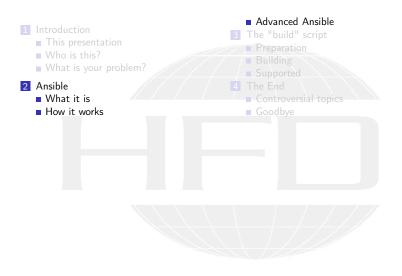
- Sometimes one needs to compile a compiler from the sources. Because
 - the compiler on the system is too old for OpenFOAM
 - a different compiler is needed. For development. Bug reproduction. Because.
- Then additional steps are needed
 - 1 Download the compiler sources
 - 2 Download additional library sources
 - 3 Extract everything in the right places
 - 4 Edit the compiler setting
 - 5 Run the compiler script in ThirdParty
- Boring. Repetitive

Introduction

The "build" script

The End

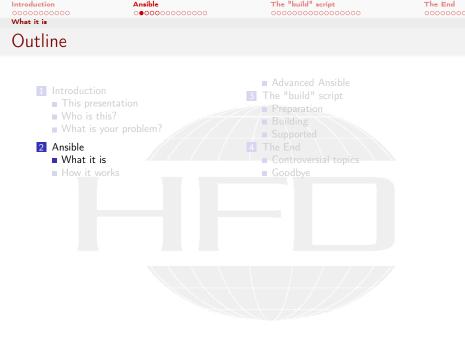
Outline



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Graz, 2019-07-03 14 / 53

Introduction 0000000000 What it is Ansible

The "build" script

The End

Wikipedia says

Ansible is an open-source software provisioning, configuration management, and application-deployment tool

In other words:

- A tool to set up computers automatically
 - Especially remote computers
 - Which computers are set up is listed in an inventory
- Setup is written in *playbooks*
 - Stored on the management machine
- Similar packages are Puppet, CfEngine and Chef
 - But they need special *Agents* on the target machines

Basically: you write how the environment should look like and Ansible tries to make it look that way

- Around since 2012
 - The developing company is part of RedHat since 2015
- Written in Python

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Introduction 00000000000 What it is Ansible

The "build" script

The End 0000000000

What it can do

There is a lot of modules but the most important ones do

- install software
- create files, directories and links (and set their attributes)
- create users and groups
- edit files (add lines, remove lines)
- manipulate source control repositories
- download files (and check their integrity)
- copy files to the remote machine

Implemented in such a way that subtle difference between distros don't matter

and if all else fails it executes regular commands

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Introduction 00000000000 What it is The "build" script

The End 0000000000

What it requires

On the master

- Ansible
 - Which needs Python
- An ssh client
- On the target machines
 - Python
 - A ssh server
 - No Ansible

Except for Ansible this is pretty standard on Linux machines

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Introduction 00000000000	Ansible 00000 000000 000	The "build" script 000000000000000000000000000000000000	The End
How it works Outline			
 Introduction This pres Who is the what is y Ansible What it is How it we have it	entation nis? /our problem? s	 Advanced Ansible The "build" script Preparation Building Supported The End Controversial topics Goodbye 	

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 Ansible

The "build" script

The End

YAML: Python of file formats

- OpenFOAM was written in C++
 - The file format looks like C++
 - With ; { }
- YAML looks like Python
 - Indentation is important
 - Less "special" characters
 - More lines

YAML

number: 2
name: foo
text: "Longutext"
list:
- one
- two
dict:
a: 1
b: 2

OpenFOAM

number 2;
name foo;
<pre>text "longutext";</pre>
list (one two);
dict {
a 1;
b 2;
1

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Introduction 0000000000 How it works The "build" script

The End

Jinja: Templates

- Jinja is a template language
 - Templates are files where "special" regions are replaced with calculation results
 - All other formatting is preserved
 - The "special" region in Jinja is between {{ an }}
 - There are also "programming" constructs like {% for %} and {% if %}

Template

```
{% for a in [1,2,3,4,5] %}
- Square of {{ a }} is {{ a*a }}
{% endfor %}
{% if x is not defined %}
No x
{% - else %}
x is {{x}}
```

Result	

	oquaro	· · ·	-	10	-
-	Square	of	2	is	4
-	Square	of	з	is	9
-	Square	of	4	is	16
-	Square	of	5	is	25

No x

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Introduction 00000000000 How it works Ansible

The "build" script

The End 0000000000

Specifying how the world should be

- Ansible does this in playbooks
 - These are YAML-files with Jinja-expressions
- Parts of playbooks

hosts On which machine should this be executed vars pre-defined variables

tasks main part. A list of tasks. A task has

name A readable name that is reported copy / file / lineinfile / debug Name of the module which is a dictionary with its parameters.

register Save the result of the task to a variable when condition to switch the task on and off

Ansible supplies variables with information about the system

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 Ansible

The "build" script

The End

Creating and editing a file

The playbook

```
hosts: localhost
      vars:
                fname: foo
      tasks:
     - name: "Create ... {{fname}}...in ... / tmp"
                  copy:
                               src: "/etc/passwd"
                             dest: "/tmp/{{fname}}"
                               force: no
                  register: target
     - name: "Mark__my__entry"
                  lineinfile:
                             path: "{{target.dest}}"
                               line: "******..we..are..here..*****"
                               insertbefore: "^{{ansible_user_id <brk>
                                                               <cont> }}:"
                  register: insert
     - name: "Report usuccess"
                  debug:
                            msg: "Modified, {{target.dest}}, on <br/> <br/> // on <br/> // on <br/> 
                                                                <cont>u {{ ansible_nodename }} "
                when: insert.changed
```

What it does

- Copies the contents of /etc/passwd to /tmp/foo
- Searches for the entry of the current user
 - Inserts a "marker" line before that if there is none
- If a line was inserted it prints a message

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Introduction 00000000000 How it works

Run it once

Ansible

The "build" script

The End

The command ansible-playbook executes the playbook

```
> ansible-playbook setLine.yml
[WARNING]: provided hosts list is empty, only localhost is available. Note that the <br/>
   <cont>implicit localhost does not match 'all'
ok: [localhost]
changed: [localhost]
changed: [localhost]
ok: [localhost] => {
  "msg": "Modified /tmp/foo on bg-postmac-budgie"
3
PLAY RECAP ***************
            : ok=4 changed=2 unreachable=0 failed=0
localhost
```

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Introduction 00000000000 How it works Ansible

The "build" script

The End 0000000000

Now everthing is good

Running it a second time doesn't change anything

This is called idempotence

```
> ansible-playbook setLine.yml
[WARNING]: provided hosts list is empty, only localhost is available. Note that the <br/> <br/> <br/> (brk>
   <cont>implicit localhost does not match 'all'
ok: [localhost]
ok: [localhost]
ok: [localhost]
skipping: [localhost]
localhost
          : ok=3
             changed=0 unreachable=0 failed=0
```

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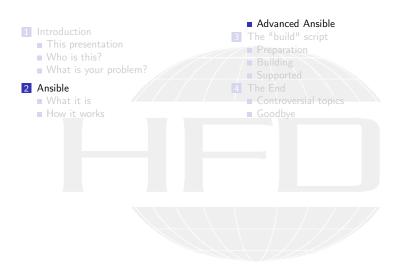
Introduction 00000000000 Advanced Ansible

Outline

Ansible

The "build" script

The End



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Introduction 00000000000 Advanced Ansible Ansible 00000000000000000000 The "build" script

The End

Roles

- Ansible-roles are usable like regular modules
 - Can have parameters
- Organized in a special directory structure with
 - Tasks
 - Variable files
 - Data files (including templates)
 - Information about dependencies
 - roles that are automatically run before running the tasks in this role
- All the tasks of the *build script* are organized in roles

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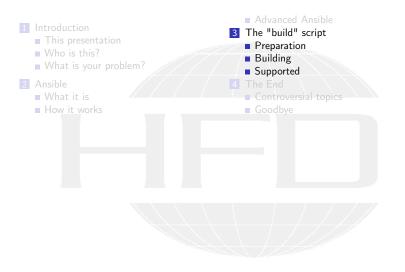
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Introduction

The "build" script

The End

Outline



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Introduction

The "build" script

The End 0000000000

Organization

- The "build script" is organized as a couple of *roles* that depend on each other
 - Before the role openfoambuild can build OpenFOAM it needs openfoamdir
 - Before openfoamdir can create a proper directory structure in needs openfoamrequirements
 - openfoamrequirements makes sure everything needed for the build is there
- The user writes a little playbook that specifies
 - Which OpenFOAM-version he wants
 - How they should be built
- Executing the playbook does everything else

The following slides explain what is done not how it is done

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Introduction Operation Outline Ansible 000000000000000 The "build" script

The End



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The "build" script

The End 0000000000

Creating a openfoam-user

- This is the user that "owns" the OpenFOAM-installation
 - Not a "normal" (human) user
 - But it should not be root
- It is made sure that such a user-exists
 - A different name can be selected
 - Name of the current user if no "special" user is desired
 - But you can name him fluent as well

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Graz, 2019-07-03 30 / 53

Introduction 00000000000 Preparation The "build" script

The End

Installing requirements

This part makes sure that required software is installed like

- Developer tools (compilers etc)
- System tools (sudo)
- Source control tools (git and mercurial)
- Development libraries (zlib etc)
- MPI-implementations
- It assumes that this is a vanilla installation
 - Minimal installation of the Linux distro
 - Nothing is there
 - Adds software repositories
- This is the part that strongly depends on the Linux-distro
 - Switches to the correct playbook depending on the distro

The "build" script

The End 0000000000

Creating a OpenFOAM-directory

- OpenFOAM usually assumes that it is in a directory OpenFOAM in \$HOME
 - Directory foam for foam-extend
- Script creates that directory
 - Make openfoam the owner
 - Adds a site directory for config files
 - A symbolic link foam pointing to it
- openfoambuild will add the proper sub-directories to it

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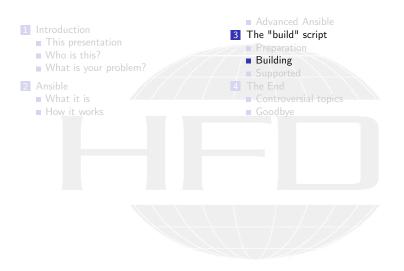
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Graz, 2019-07-03 32 / 53

Introduction Occorrection Building

The "build" script

The End



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Introduction 00000000000 Building The "build" script

The End 0000000000

What it does

Downloads the correct sources (ThirdParty as well)

- Either a tarball
- a git archive
- Extracts the sources to the correct directories
- Puts the sources under version control (optional)
- Applies patches
- Runs the compilation script
 - If this is successful the script will not be run again
- All this is controlled by settings for each distro in a dictionary distros
 - Settings can be overwritten per Linux-distro (because of different requirements) in distroarch

Introduction 00000000000 Building Ansible 000000000000000 The "build" script

The End 0000000000

Example for a distro-specification

From defaults/main.yml	
p1906:	
name: OpenFOAM-v1906	
# where to load the sources from. Only used if 'gitrepo' is undefined	
tarball: https://sourceforge.net/projects/openfoamplus/files/v1906/Open <cont>v1906.tgz</cont>	nFOAM- <i><brk></brk></i>
# tarball is checked against this checksum before extracting	
tarballcheck: md5:ab7017e262c0c0fceec55c31e2153180	
# tarball with the ThirdParty-Sources. If no repo is defined	
tarball3rd: https://sourceforge.net/projects/openfoamplus/files/v1906/	<brk></brk>
<cont>ThirdParty-v1906.tgz</cont>	
tarball3rdcheck: md5:81af204ef7aa804bc6b633f20f28749e	
name3rd: ThirdParty-v1906	
thirdParty: - metis51	
version: v1906	
# The API version that was introduced in $v1812$	
api: "1906"	
hasBuildDir: True	

This is all that had to be added to support OpenFOAM v1906

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Introduction 00000000000 Building The "build" script

The End 0000000000

Building ThirdParty

- Regular ThirdParty-sources are downloaded automatically
- Additional third party software is downloaded
 - Specified in the thirdParty-setting
 - May be different depending on the distribution
 - If there is no appropriate MPI-implementation for instance openmpi211 can be specified to get OpenMPI 2.11
- Appropriate files in OpenFOAM/site are modified to use it
- This software is automatically compiled
- Name, locations etc specified in configuration dictionary thirdParty

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Introduction 00000000000 Building The "build" script

The End 0000000000

Building compilers

- Compilers are a special case of third party software
 - Depend on multiple tarballs
 - OpenFOAM-scripts expect a special directory structure
- This is configured in compilerSpec
- If a compiler is compiled then it is made the default for this distro
 - People who use more than one compiler consider this a bug



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Graz, 2019-07-03 37 / 53

Introduction 00000000000 Building The "build" script

The End

Example for a playbook

Build a OpenFOAM-distro for development

Single command entertains the computer for a couple of hours > sudo ansible-playbook exampleConfigs/normalAndDebug.yml --extra-vars="distro=p1906"

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Introduction 00000000000 Building The "build" script

The End 0000000000

Building additional software

- There is a role openfoamdocu that builds the Doxygen-documentation
 - Makes sure that the distro is compiled
 - Installs the necessary software (doxygen, graphviz)
- Roles for selected software packages

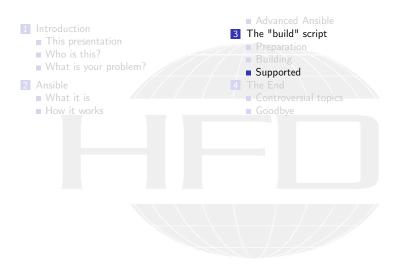
cfmesh for distros that don't bring this swak4foam The *Swiss Army Knife For OpenFOAM*. No machine should be without this pyfoam Python library and utilities for OpenFOAM

- These roles
 - Make sure that the distro is compiled
 - Install into a special AdditionalSoftware-directory for every distro separately

Introduction		
00000000000		
Supported		
Outline		

The "build" script

The End



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Introduction 00000000000 Supported The "build" script

The End

How to get it

- The "Homepage" of the script is https: //openfoamwiki.net/index.php/Installation/Ansible
- Easiest way to get it: Mercurial

Download

```
> hg clone http://hg.code.sf.net/p/openfoam-extend/ansibleFoamInstallation
> cd ansibleFoamInstallation
```

Further documentation in the README

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Graz, 2019-07-03 41 / 53

Introduction 00000000000 Supported The "build" script

The End 0000000000

Supported OpenFOAM forks

The three forks are supported in their latest versions OpenFOAM Foundation Version 6. Expecting 7 in the next month OpenFOAM ESI / Plus Version 1906 Foam Extend the nextRelease (Version 4.1) branch Older versions as well (check the documentation)



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Introduction Supported

Ansible

The "build" script The End

Supported Linux distributions

Tested distros are CentOS / RedHat Version 6 and 7 Ubuntu The LTS-versions 18.04 and 16.04 ArchLinux / Manjaro Because this is a rolling distro it is not 100% stable Implemented but not tested in a long time Fedora last I checked was 25 Darwin Not a Linux. And software installation has to be done by hand AlpineLinux Not yet completed

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Heinemann Fluid Dynamics Research GmbH Graz. 2019-07-03

43 / 53

Outline	
Outline	
Outline	
 Introduction This presentation Who is this? What is your problem? Ansible What it is How it works 	 Advanced Ansible The "build" script Preparation Building Supported The End Controversial topics Goodbye

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The End

Ansible 000000000000000000000000000000000000	The "build" script	The End
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Graz, 2019-07-03 45 / 53

Introduction **Controversial topics**

The user

Ansible

The "build" script

Some sysadmins think that creating a user is a bit intrusive. So

- If you're in an environment with a directory service (LDAP etc): create the user there by hand because this Ansible-script will create only local users
- There is an additional variable for a openfoam-group. But that is optional

Can be nice if you want all OpenFOAM-users in that group



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46 / 53

Introduction Controversial topics Ansible

The "build" script

The End

The location

- With the standard-settings a directory /home/openfoam/OpenFOAM is created
 - Everything will go into that directory
 - Make sure it is on a drive with sufficient space
- It is recommended to move this to an appropriate location
 - and set a symlink
 - But this has not been "ansibled" because it depends on the specific environment



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47 / 53 Graz. 2019-07-03

Introduction 0000000000 Controversial topics Ansible 000000000000000 The "build" script

The End

Superuser rights

- Certain operations (package installation) require super-user rights
 - Also: "becoming" user openfoam
- So usually the playbooks have to be run with sudo



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Graz, 2019-07-03 49 / 53

Introduction Goodbye

Ansible

The "build" script

The End 00000000000

Contributions

- Contributions are most welcome
- Especially support of new Distros
 - Also Windows if you want to
- Testing of the unsupported ones
- If somebody wants to write a role to compile ParaView: great



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50 / 53

Introduction 00000000000 Goodbye Ansible 000000000000000 The "build" script

The End

No questions

Thanks for listening Suggestions? Comments? Offers for help?

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Graz, 2019-07-03 51 / 53

Introduction 00000000000 Goodbye The "build" script

The End

OpenFOAM Workshop

See you in Duisburg later this month (23rd to 26th)



http://openfoamworkshop.org/

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Introduction 00000000000 Goodbye The "build" script

The End

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Bernhard F.W. Gschaider original author and responsible for the strange English grammar. Contact him for a copy of the sources if you want to extend/improve/use this presentation

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