DAPHNE 4NEDI

User Centric Key Drivers:

- Software Quality:
 - Functional attributes: Rich feature set addressing Use Cases, defect free.
 - Non functional attributes: Stability/Reliability, high performance, efficiency in use of system resources, usability.

Agile Software Development

- Responsive/Adaptable to User needs, faster turnaround times, *always working software*.
- Overcome Integration Hell of bulk code integration of Waterfall model.
- Overcome *Dependency Hell* with software packaging techniques.

• DAPHNE TA3

- Curated Repository of Data Analysis Software & Datasets based on FAIR principles with *Re-usability* focus for Power Users and User community at large.
- Usability: User's simply run S/W out of the box, and get their job done without worrying about installation & configuration.
- High Quality Software = Widespread adoption / Large user base.

Risk factors for defects creeping during Integration (Integration Hell)

- **Size of Code Changes**: The larger the code change, the higher the chance of introducing defects. Mistakes in merging, refactoring, logic, syntax, or (requirements) implementation.
- **Unfamiliarity with the Code**: Misunderstand logic, miss dependencies, or introduce inefficiencies (duplication).
- **Depth of Code Changes**: Changes deep into core logic, infrastructure, or low-level dependencies, the risk is much higher.
- Code Complexity/Organization: Non modular, Unintended Side Effects.
- **Dependencies & External APIs & Environment**: Not pinning versions, bundling issues.
- **Developer Team Size**: Merge conflicts, inconsistent coding styles, and integration issues.
- Incomplete Testing: Insufficient test coverage.

Coding Standards,Git Commit Guidelines, Peer review, Code Inspection with Static Code Analysis tools and various levels of Testing improve Software Quality.

Risks in packaging & deployment (Dependency Hell)

- Source distribution puts unnecessary overhead of replication of build environment on users.
- Version conflicts at OS package level (needed vs. installed).
- Version conflicts between at programming language package manager level (need vs. installed).
- Elevated privileges requirement.





Practices supported by tools

- **Continuous Integration**: Frequent build, unit, integration, regression tests & packaging of each small change/commits to detect defects early.
- **Continuous Delivery**: Frequent integrity checks, system tests, security scanning of packages and publishing in repositories for *manual* deployment.
- **Continuous Deployment**: Frequent *Automatic* deployment of packages in production from the repositories.
- Automation tools:
 - Repetitive & reproduce-able CI/CD, provide fast feedback and free us to work on non-repetitive tasks.
 - Custom build rigid build script of the past is now very configurable.
 - UI Dashboard to visibility and control of CI/CD process.





Continuous Integration & Delivery/Deployment at DESY FS-SC Gitlab CI/CD activities GitLab

- Windows 11 • Installation and Configuration of Windows and MacOS (15.3.1Sequoia) Runners.
- Updated CI/CD for :
 - CrystFEL
 - Container builds for Fedora, Ubuntu, AlmaLinux.
 - Singularity/Apptainer container image using Kaniko.
 - Homebrew recipe for MacOS.
 - Continuous deployment on Maxwell. 逆
 - Nuclear Elastic X-ray scattering Universal Software (Nexus) nexus
 - Windows 11 and MacOS builds
 - Many linux dynamically linked Python 3.6 3.12 container image.
 - Pyinstaller executables using Many Linux containers.
 - Plug2: A simple plotter for XPCS @P10
 - RSAP: Reciporcal Space Maps Program
 - For building FS-EC Tango debian packages.















Pyinstaller the Python Packaging tool

- Generates a single, self extracting executable.
- Isolated /Insulated/Standalone/Sandboxed runtime environment.
- Bundle of Python program, language and system libraries and all resources.
- Supports different operating systems: Linux, Windows, Mac.
- Used Gitlab & Many Linux to build binaries on wide range of Linux.



Core Concepts

- **Pipeline**: The entire CI/CD workflow executed on code changes. (.gitlab-ci.yml)
- Stage: Logical grouping of jobs (e.g., build, test, deploy).
- Job: A task executed in a pipeline stage.
- Runner: The machine that executes jobs.
- Artifact: Files (e.g., binaries, logs) saved after a job.
- Cache: Reusable dependencies to speed up pipelines.



Keyword	Purpose	Example
stages	Defines pipeline stages	<pre>stages: [build, test, deploy]</pre>
jobs	Defines tasks in a stage	build_job:
before_script	Prepares the environment	before_script: [apt update]
script	Runs job commands	script: [make build]
after_script	Executes cleanup tasks	after_script: [rm -rf tmp]
artifacts	Stores job output files	<pre>artifacts: { paths: ["dist/*"] }</pre>
cache	Reuses dependencies	<pre>cache: { paths: ["node_modules/"] }</pre>
dependencies	Controls which artifacts a job downloads	dependencies: ["build"]
only/except	Specifies when jobs run	only: [main]
rules	Controls when jobs run	rules: - if: '\$CI_COMMIT_BRANCH == "main"'
when	Controls job execution	when: manual
image	Defines the Docker image	image: python:3.9
services	Adds additional containers	services: [mysql:latest]

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CrystFEL

- Open source C/C++ code base.
- Source distribution for various Linux flavours and MacOS (with also Homebrew Recipe) Docker image, Apptainer "def file".
- Cmake, Meson and Ninja build tools.
- Prerequisite External dependencies: Features set dependent on other libraries used at build time.
 - HDF5,HDF5 External plugin (Nexus format), GSL, FFTW, MSG Pack, ZMQ.
 - Leverage a binary library platform specific distribution where available.
 - Otherwise, build a library package from source.
- Build, unit test and install locally.

Earlier CrystFEL Maxwell deployment approach

- Daily cron job (shell script *run-me*) on a Maxwell node and an user account.
- One time install of build tools: *Python, meson* and *ninja*.
- Build & install steps in *run-me* script:
 - Clean target directory /software/crystfel/devel
 - Download and install *cmake* from binary distribution.
 - Download other external dependencies source tarballs and build and install libraries under */software/crystfel/devel*. HDF5, HDF5 External plugin (Nexus format), GSL, FFTW, MSG Pack, ZMQ.
 - Clone CrystFEL source code from Gitlab master branch.
 - Build CrystFEL and install locally at /software/crystfel/devel.
- Disadvantages:
 - Scheduled daily build and install even when there is no change to CrystFEL code base.
 - Risk of broken installs.

Revamped CrystFEL CI/CD

- Multiple stages with their jobs Build, Test, Deploy, Build Container.
- Manual stage for building Dev Environment container images with all dependencies.
- Gitlab CI/CD pipeline triggers the builds on merge to master branch.
- All jobs run on different runners Gitlab kubernetes cluster, MacOs.
- Maxwell build stage job now runs under AlmaLinux9 container in Gitlab kubernetes cluster.
- Deployment stage job:
 - Remotely copy (scp/rsync) the built software onto Maxwell target directory /software/crystfel/devel.
 - Authentication using ssh private key/public key pair or Kerberos.
 - Run under CentOS container in Gitlab kubernetes cluster.
- Advantages:
 - Installs only *on change* to source code base that build & undergo unit test successfully.
 - Complete visibility in Gitlab CI/CD pipeline & audit trail.
 - Dev Env images have cut the build & deployment time from 25 mins to 8 mins. ¹⁷

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114	GIT_STRATEGY: clone
115	script:
116	- brew uninstall -v -f crystfel
117	- brew install -v -s ./crystfel.rbHEAD
118	- brew test crystfel
119	- brew uninstall -v -f crystfel
120	rules:
121	<pre>- if: \$CI_COMMIT_BRANCH == "master"</pre>
122	
123	deploy-remote-maxwell:
124	stage: deploy
125	<pre>image: \$CI_REGISTRY_IMAGE/alma9</pre>
126	dependencies:
127	- "build-and-test: [alma9]"
128	variables:
129	GIT_STRATEGY: clone
130	tags:
131	- DESY-intern
132	before_script:
133	##
134	## KUN SSN-Agent (Inside the Duild environment)
135	## Give the right permissions, otherwise son-ada will refuse to add files
130	## Adu the son key stored in MAAWELL_SON_PRIVALE_KET File type ti/to variable to the agent store
130	WW Greate the son directory and give it the right permissions while Maywell SCH Delivere Vevic pot cot theory of Maywell DEED NAME and MAYWELL ACCOUNT DASCWARD
130	"" 1; IMAMELL_JOST_TAIVATE_RET IS HUL SEL LHEH USE \$MAAMELL_USER_MARE WHU \$MAAMELL_ALLUUNI_PASSWURU
140	- UCT- move-ware .
140	- PRFFTX="=]ma0".
142	- if [\$MAXWELL SSH PRIVATE KEY]: then
143	eval \$(ssh-acent -s);

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D 13	12	123	deploy-remote-maxwell:
0.0.1		124	stage: deploy
Q Search or g	go to	125	image: \$CI_REGISTRY_IMAGE/alma9
		126	dependencies:
roject		127	- "buld-and-test: [alma9]"
-		128	
CrystFEL		129	GII_SIRATESY: CLONE
A Discost		130	Lags:
r Pinnea	~	132	before conjunt:
lesues	25	133	##
100000		134	## Run ssh-agent (inside the build environment)
Merge requests	0	135	## Give the right permissions, otherwise ssh-add will refuse to add files
		136	## Add the SSH key stored in MAXWELL_SSH_PRIVATE KEY file type CI/CD variable to the agent store
Pipelines		137	## Create the SSH directory and give it the right permissions
		138	## If MAXWELL_SSH_PRIVATE_KEY is not set then use \$MAXWELL_USER_NAME and \$MAXWELL_ACCOUNT_PASSWORD
8 Manage	>	139	## to connect using Kerberos.
Diana		140	- HOST="max-wgs";
I Plan	>	141	- PREFIX="alma9";
D Code	、 、	142	- if [\$MAXWELL_SSH_PRIVATE_KEY]; then
, coue		143	eval \$(ssh-agent -s);
🛿 Build	>	144	chmod 400 "\$MAXWELL_SSH_PRIVATE_KEY";
		145	<pre>ssh-add "\$MAXWELL_SSH_PRIVATE_KEY";</pre>
D Secure	>	146	else
_		147	echo \$MAXWELL_ACCOUNT_PASSWORD kinit \$MAXWELL_USER_NAME@DESY.DE;
Deploy	>	148	
D. Onerete		149	conjet
operate	,	150	soript. - denlayment/denlay-ta-maywell sh "\$MAYWELL USED NAME" "\$UAST" "\$PRETY"
Monitor	>	151	deproymency deproy to manifection grandle_ooth_name groot grant a
E montor		153	rules:
과 Analyze	>	154	- if: \$CI_COMMIT_BRANCH == "master"
-		155	
		156	build_container_image:
		157	stage: build_container
		158	dependencies: []
		159	only:
		160	- master
		161	image:
		162	name: gcr.io/kaniko-project/executor:debug
		163	entrypoint: [""]
		164	
		165	
		100	IMAGE: "Crystrel"
		107	INAGE IAG_LAIESI: "Latest"
		108	DOCKEP HOST top://docker:3375
		170	DOCKER TIS CERTITE: ""
		171	
		172	script:
		173	- echo "{\"auths\":{\"\$CI_REGISTRY\":{\"username\":\"\$CI_REGISTRY_USER\",\"password\":\"\$CI_REGISTRY_PASSWORD\"}}}" > /kaniko/.docker/config.1
		174	
Dinetp		175	/kaniko/executor
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D> มีว	⊡ 12	155	
		156	build_container_image:
O Search or go t	to	157	stage: build_container
		158	dependencies: []
Droject		159	
Project		100	- <u>I</u> master
CrystEEI		161	image:
CIVSUEL		162	entrypaints [""]
🖍 Pinned	~	164	
		165	variables:
Issues	25	166	IMAGE: "crystfel"
M	0	167	IMAGE_TAG_LATEST: "latest"
Merge requests	0	168	IMAGE_TAG_SHA: \$CI_COMMIT_SHORT_SHA
Pipelines		169	DOCKER_HOST: tcp://docker:2375
		170	DOCKER_TLS_CERTDIR: ""
86 Manage	>	171	
<u> </u>		172	script:
🔁 Plan	>	173	<pre>- echo "{\"auths\":{\"\$CI_REGISTRY\":{\"username\":\"\$CI_REGISTRY_USER\",\"password\":\"\$CI_REGISTRY_PASSW0RD\"}}}" > /kaniko/.docker/config.j</pre>
		174	- >
Code	>	175	/kaniko/executor
		176	context \$C1_PR0JECT_DIR
Build	>	177	dockertile \$CI_PRUJECI_DIR/deployment/dockertile
T Sacura		178	destination \$L_REDISTRY_IMAGE/\$IMAGE:ADDATE TAG
V Secure		179	destination sul_keois kt_inade; sinade: sinade: adosha
Deploy	>	181	build-ang harty version-shelm_version
<u> </u>		182	bold any KANONEK_UCI_VEROIDA-\$KANONEK_UCI_VEROIDA
Operate	>	183	tags:
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Lh. Amelume		186	when: manual
🕮 Anatyze	>	187	
		188	build_container_image_tag:
		189	stage: build_container
		190	image:
		191	name: gcr.io/kaniko-project/executor:debug
		192	entrypoint: [""]
		193	vani obligati
		194	Variables.
		195	TIMOL STATES
		190	DOCKER HOST: top://docker:2375
		198	DOCKER TLS CERTDIR: ""
		199	
		200	script:
		201	<pre>- echo "{\"auths\":{\"\$CI_REGISTRY\":{\"username\":\"\$CI_REGISTRY_USER\",\"password\":\"\$CI_REGISTRY_PASSW0RD\"}}}" > /kaniko/.docker/config.j</pre>
		202	- >
		203	/kaniko/executor
		204	context \$CI_PROJECT_DIR
		205	dockerfile \$CI_PROJECT_DIR/deployment/docker/Dockerfile
		206	destination \$CI_REGISTRY_IMAGE/\$IMAGE:\$IMAGE_TAG_VER
(?] Help		207	build-arg HELM_VERSION=\$HELM_VERSION
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Monitor	Trigger a pi	ipeline for a branch or tag by genera	ating a trigger toker	n and using it wi	th an API call. The token in	personates a											
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THelp

Filter pipelines				Q Show Pipeline ID ~
Status	Pipeline	Created by	Stages	Action
 ✔ Passed ③ 00:04:21 ≅ 2 days ago 	align_detector: Skeleton code for showing mea #163039 ٷ show-mille-measurements ☞ 01bb9543 ☺ latest	•	0	ج بر ج
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 ★ Failed ③ 00:03:27 ☐ 1 week ago 	Merge branch 'fix-fg-graph-round' into 'master' #160127 ♀ master ໍ ↔ dcfab39d 😧		(w)- <mark>(3)</mark> - (w)- (w)	~ به <
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Q Search or	go to	1045 Installing /builds/thomas.white/crystfet/data/crystfet.svg to /software/crystfet/devet/snare/icons/nicotor/scatable/apps	
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23 0.90.00		1650 Installing symlink pointing to libcjson_utils.so.1.7.15 to /software/crystfel/devel/lib64/libcjson_utils.so.1	Queued: 1 sec
🔊 Pinned	~	1651 Installing symlink pointing to libcjson_utils.so.1 to /software/crystfel/devel/lib64/libcjson_utils.so	Timeout: 1h (f
lecuoc	25	1652 Installing symlink pointing to libcrystfel.so.18 to /software/crystfel/devel/lib64/libcrystfel.so	Pupper: #215
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Merge requests	s 0	1654 \$ echo '#!/bin/sh' > \$CFPREFIX/bin/crystfel	rke2)
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88 Manage	,	1657 \$ chmod +x \$CFPREFIX/bin/crystfel	Job artifacts (
		1658 \$ mv \$CFPREFIX/bin/get_hkl \$CFPREFIX/bin/get_hkl.real	These artifacts
🔁 Plan	>	1659 \$ echo '#!/bin/sh' > \$CFPREFIX/bin/get_hkl	not be deleted
		1660 \$ echo "export SYMINF0=\$CFPREFIX/share/ccp4/syminfo.lib" >> \$CFPREFIX/bin/get_hkl	newer artifacts
Code	>	1661 \$ echo "\$CFPREFIX/bin/get_hkl.real \"\\$@\"" >> \$CFPREFIX/bin/get_hkl	Keep
Ø Build	~	1662 \$ chmod +x \$CFPREFIX/bin/get_hkl	Reep
D Duite		1663 \$ wget -nv <u>https://www.mrc-lmb.cam.ac.uk/mosflm/wosflm/ver740/pre-built/mosflm-linux-64-noX11.zip</u>	
Pipelines		1664 2025-02-21 16:36:58 URL: <u>https://www.mrc-lmb.cam.ac.uk/mosflm/mosflm/ver740/pre-built/mosflm-linux-64-noX11.zip</u> [4588319/4588319] -> "mosflm-linux-64-noX11.zi	Commit 01bb9
I Jaka		p" [1]	align_detector:
JODS		1665 \$ unzip mosflm-linux-64-noX11.zip	ng measureme
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		1667 inflating: mosflm-linux-64-noX11	Pipeline #1630
Pipeline schedu	ules	1668 \$ mv mosflm-linux-64-noX11 \$CFPREFIX/bin/mosflm.real	w-mille-meas
Artifacts		1669 \$ echo '#!/bin/sh' > \$CFPREFIX/bin/mosflm	
-		1670 \$ echo "export SYMINFO=\$CFPREFIX/share/ccp4/syminfo.lib" >> \$CFPREFIX/bin/mosflm	test
Ø Secure	>	1671 \$ echo "\$CFPREFIX/bin/mosflm.real -n \"\\$@\"" >> \$CFPREFIX/bin/mosflm	
Doplay		1672 \$ chmod +x \$CFPREFIX/bin/mosflm	Related jobs
C ⁴ Depiloy		1673 \$ cp -Rp /software \$CI_PROJECT_DIR/\$PLATFORM	build
Operate	>	✓ 1674 Uploading artifacts for successful job 81:80	S Duita
		1675 Uploading artifacts	→ 🙆 build
💮 Monitor	>	1676 alma9: found 1357 matching artifact files and directories	
hu Apolyzo	、 、	1677 build/meson-logs/testlog.junit.xml: found 1 matching artifact files and directories	🕝 build
- Anatyze		1678 Uploading artifacts as "archive" to coordinator 201 Created 1d=711695 responseStatus=201 Created token=glcbt-64	-
		16/7 Uploading artifacts	🕑 build
		1680 build/meson-logs/testlog.junit.xml: found 1 matching artifact files and directories	
		1681 Uploading artifacts as "junit" to coordinator 201 Created id=711695 responseStatus=201 Created token=glcbt-64	🕑 build
		1682 Cleaning up project directory and file based variables 80:80	
		1683 Job Succeeded	

D 11 C	² removed deb10
Q Search or go to	📀 Passed Sabrina Sendel created pipeline for commit 039f3205 👔 10 hours ago, finished 3 hours ago
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⊌ □	+ 💮	tango-ds / GserverBuild
D 17	⊠ 12	🤞 .gitlab-ci.yml 👸 1.97 KiB Delete 🔀 🔂 🕁
Q Search or go to	o	1 stages:
Project		
G GserverBuild		4 build-package:
		6 rules:
X Pinned	~	<pre>7 - if: \$CI_PIPELINE_SOURCE == "pipeline"</pre>
Issues	0	9 - \$DEBIAN_VERSION
Merge requests	0	10 variables:
Dipolineo		11 GT_STRATEGY: clone
Pipetines		<pre>if [[\$PARENT_UPSTREAM_SECRET != \$DOWNSTREAM_SECRET]]; then exit; fi</pre>
🖧 Manage	>	14 - export TANGO_DIR=\$CI_PROJECT_DIR
		15 - export TANGO_DIR_GIT=\$TANGO_DIR
🔄 Plan	>	10 - export of characteristic strategies and the strategies of the
> Code	>	
n Build	、	19 for repo in \$ADDITIONAL_CLONES
g build	·	20 00 10 url=\$(echo \$repo awk -F ',' '{print \$1}')
Secure	>	22 dir=\$(echo \$repo awk -F ',' '{print \$2}')
Deploy	>	23 mkdir -p \$TANG0_DIR/\$dir
		24 CG \$1ANOU_ULK/\$01F
Operate	>	<pre>26 url='echo \$url/sed -e "s/^https:\////"`</pre>
👜 Monitor	>	27 url=https://gitlab-ci-token:\${CI_JOB_TOKEN}@\$url
-		28 git clone Surl
Analyze	>	30 done
3 Settings	>	31 - cd \$TANGO_DIR
		32 - rkdir - p \$TANGO_DIR/Libraries/cppserver
		<pre>34 - git clone https://gitlab-ci-token:\${CI_JOB_TOKEN}@gitlab.desy.de/tango-ds/libraries/cppserver/common</pre>
		35 - git clone https://gitlab-ci-token:\${CI_JOB_TOKEN}@gitlab.desy.de/tango-ds/libraries/cppserver/include
		36 - cd \$TANGO_DIR/Libraries 37 - pit clone bttps://pitlab.ci.token:\${CI_IDE_TOKEN}@pitlab_desv_de/tango_de/libraries/util/
		38 - cd uti; make; cd/.
		39 - PARENT_PROJECT_URL='echo \$PARENT_PROJECT_URL sed -e "s/^https:\/\///"`
		40 - PROJECT_URL="https://gitlab-ci-token:\${CI_JOB_TOKEN}@\$PARENT_PROJECT_URL" 41 - pit clone \$PON_FFT_URL
		42 - updatedb -l 0 -o \$TAN60_DIR/tango-ds.db -U \$TAN60_DIR
		43 - aklog -keytab ~/fsbldusr.keytab -principal fsbldusr
		44 - 45 if [["\$ADDITIONAL PACKAGES" - ""]]; then
		46 SPLI_PACKAGES=\$(./stringsplit.sh "\$ADDITIONAL_PACKAGES")
		47 ./gserverbuild.sh -tqs \$PARENT_PROJECT_NAME -a "\$SPLIT_PACKAGES";
		48 else
		50 fi
		51 parallel:
		52 matrix: 53 - DEFIN VERSION ["bulleave" "bookwoom"]
		54

Secure
Deploy
Operate
Monitor
Analyze



Observations/Conclusions

CI/CD tools like Gitlab:

- remove repetitive tasks, provides visibility & rapid feedback, speed up development.
- when used with static code analysis tools to improve code quality.
- allow comprehensive testing on multiple platforms & improve software robustness.
- Speed up of Gitlab CI/CD pipelines can be achieved by:
 - building Dev container images for static dependencies.
 - workflow & analysing job dependencies & caching.
- External runners required for MacOs, Windows and Linux for building special system packages.
- There is *no one size fits all* approach to packaging, depending on development language and runtime environments.
- Commit small, commit often & follow Git commit guidelins.

Acknowlegements to Developers:

- Thomas White (FS-SC)
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- Abdullah Malik (CFEL)
- Lars Bocklage (FS)
- Marcus Fleck (FS-EC)

Thank You!

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