20 - Portal Científico

Introdução

Julia Gschwend

Por que construir um portal científico?

- Fácil acesso a dados
- Registro de processos e produtos - organização
- Compartilhamento entre usuários geograficamente distribuídos
- Controle de proveniência - reprodutibilidade
- Automatização de atividades repetitivas
- Paralelização de códigos - escalabilidade - big data
- Repositório de códigos - legado
- Apoio tecnológico - pacotes, bibliotecas, ferramentas, helpdesk, etc.

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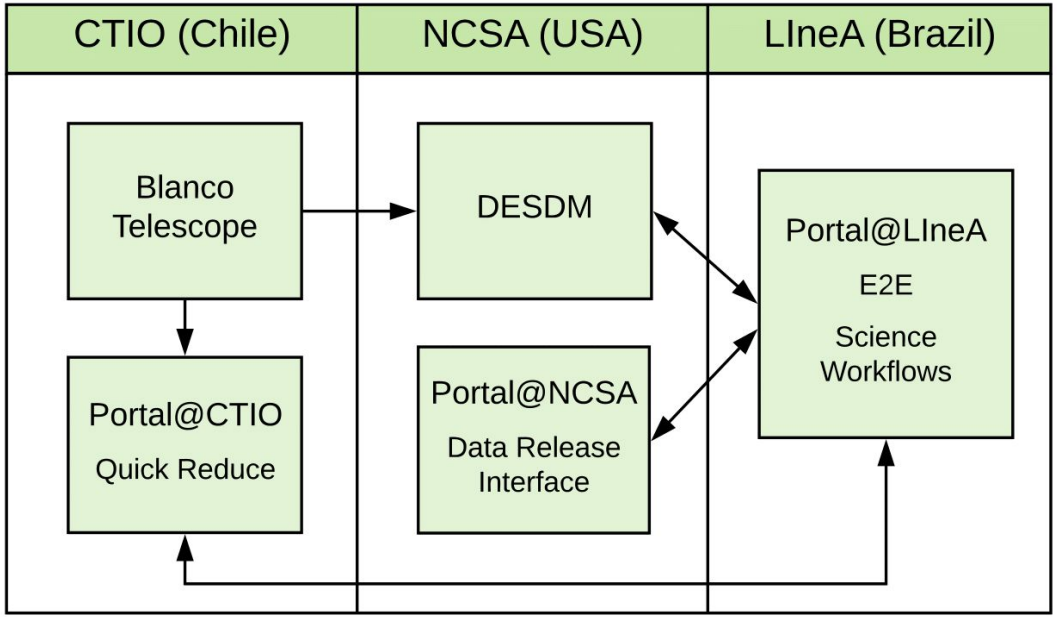
Em quais casos o portal não é indicado?

- Análise exploratória
- Desenvolvimento de pequenas aplicações
- Plots interativos

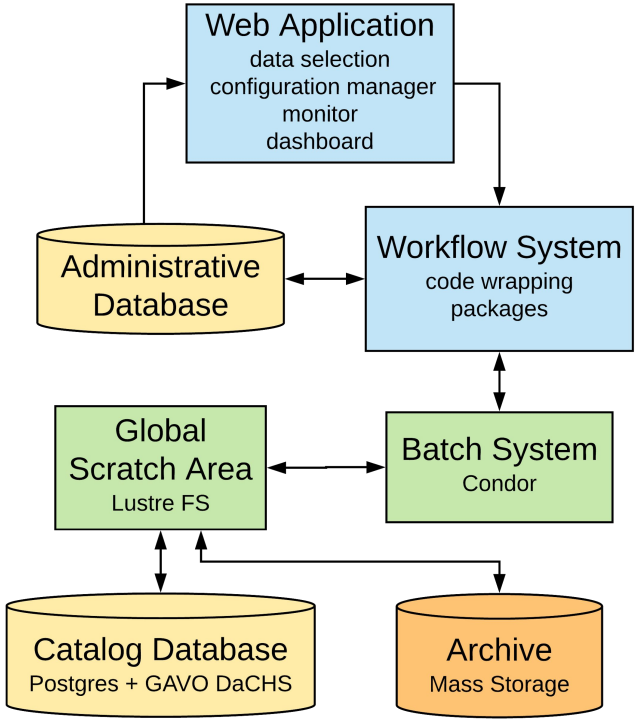
Jupyter Notebooks!!!

Instâncias do portal - dataflow

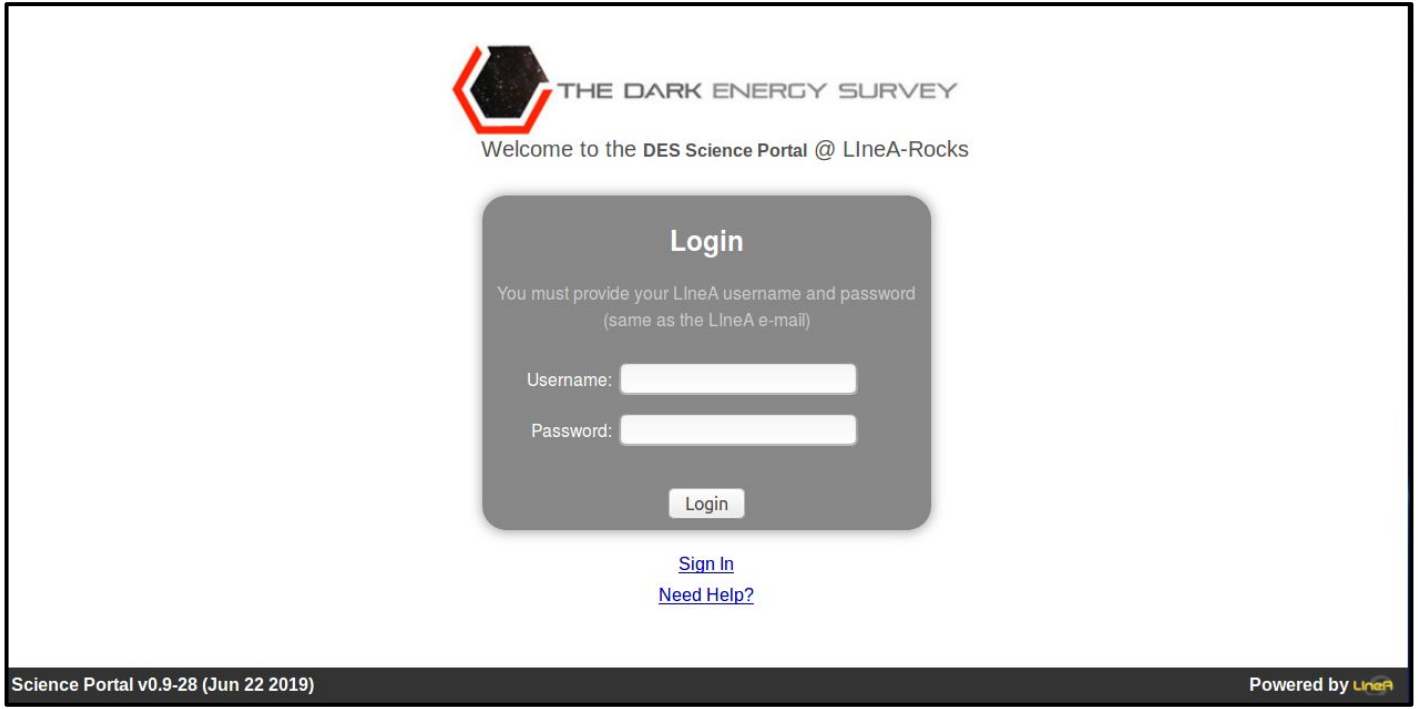


O que é o *DES Science Portal*? (@LineA)

- Front-end: interface web
  - My Workspace
  - Pipelines
  - Tools
  - Dashboard
  - Data Server
- Back-end: infraestrutura
  - 2 databases
  - Mass storage
  - Scratch area
  - Batch system
  - Workflow system
  - Computer cluster



Front-end - https://des-portal.linea.gov.br/



(demonstração ao vivo)

Pipelines & components - definições

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  - XML workflow (pipeline.xml)
  - 1 processo = 1 pipeline run

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- Organização e fluxo de dados
  - Release/dataset
    Ex.:
    Y1A1/SPT
    Y3A2/Y3 Gold Medium
    Micecat v2.0/Micecat v2.0 Small

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  - Sistema de classes
    Ex.:
    coadd_objects
    training_set
    lf_measurement

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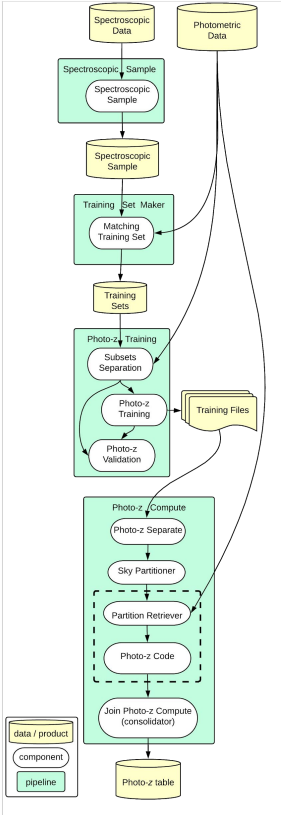

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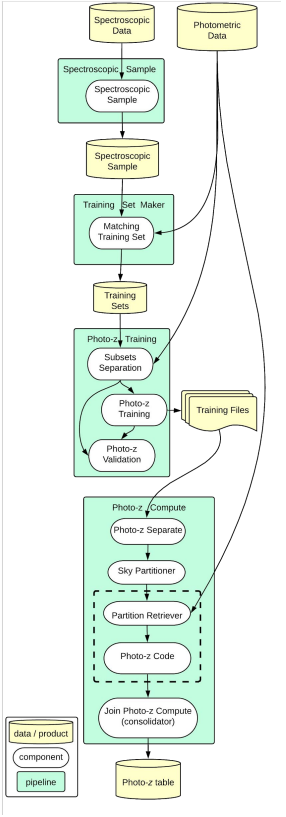
detalhes na sessão #23
(tutorial: criando um pipeline II)



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http://git.linea.gov.br/

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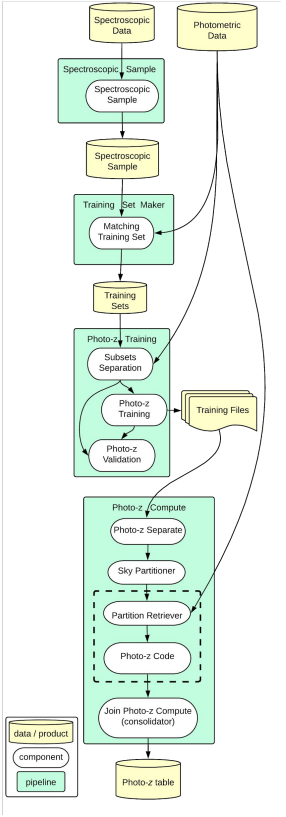
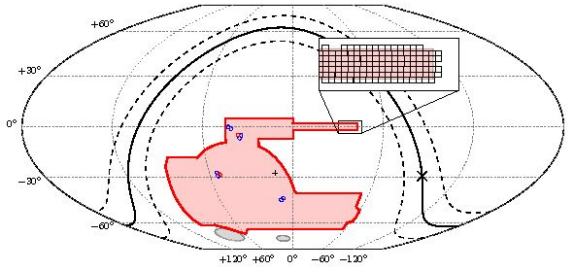
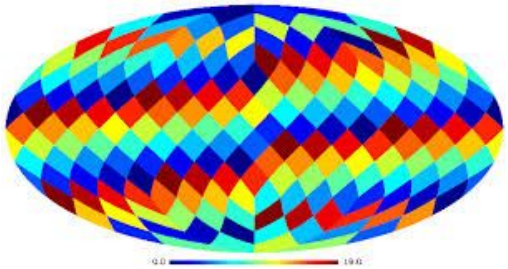
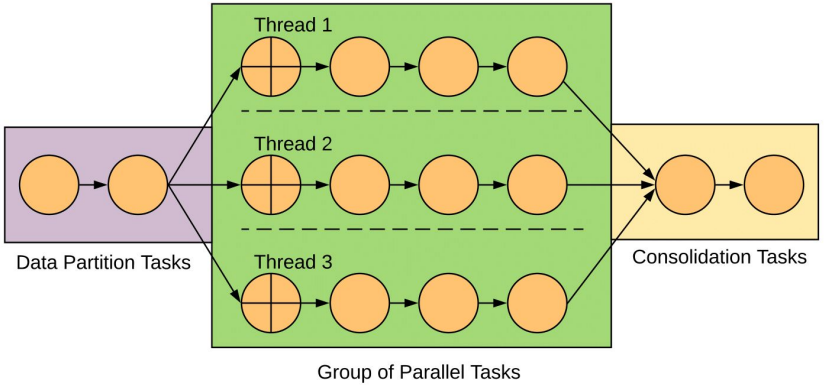


Pipelines & components - paralelização

- Paralelização tipo map & reduce
  - Espacial (~~tiles~~, HEALPix)
  - Por atributo (ex: redshift bins)
- Componentes disponíveis:
  - Dados no HDFS:
    Sky Partitioner + Partition Retriever
  - Dados no DB:
    Data Slicer + Data Retriever



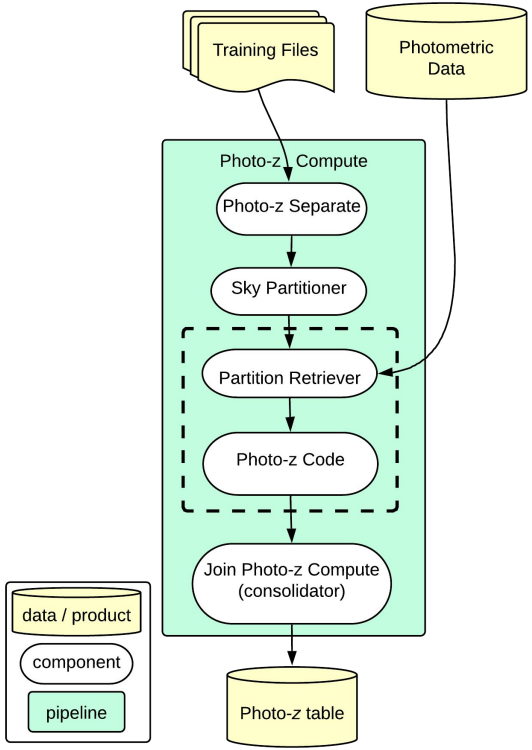




Pipelines & components - exemplo

Pipeline Photo-z Compute

- Inputs:
  - Photometric data (coadd objects)
  - Training files
- Output:
  - Photo-z table (id, z_best, z_err)
- Configurações
  - de paralelização (flexível)
  - do código (herdada via provenance)



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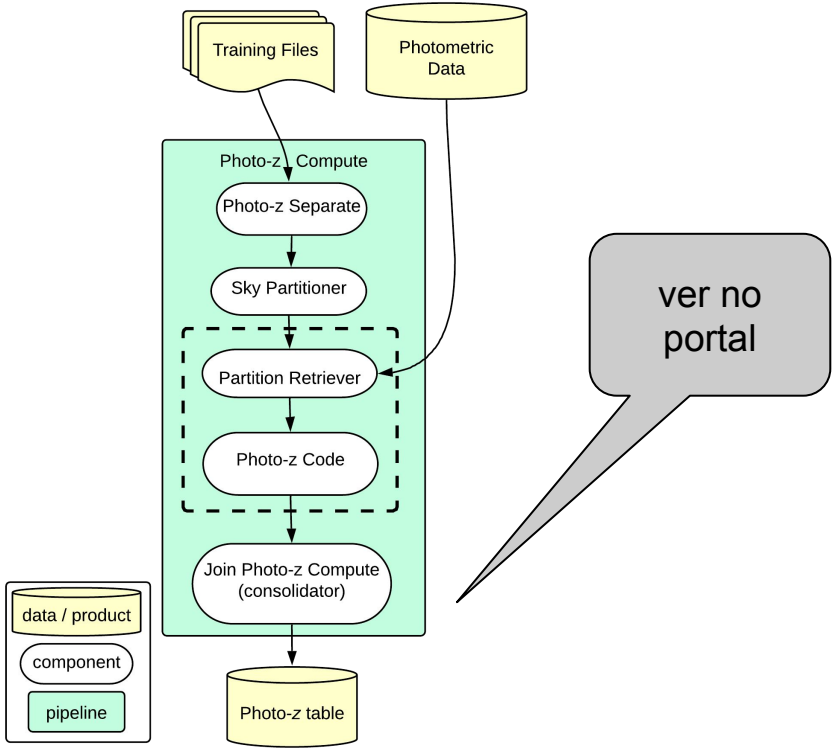
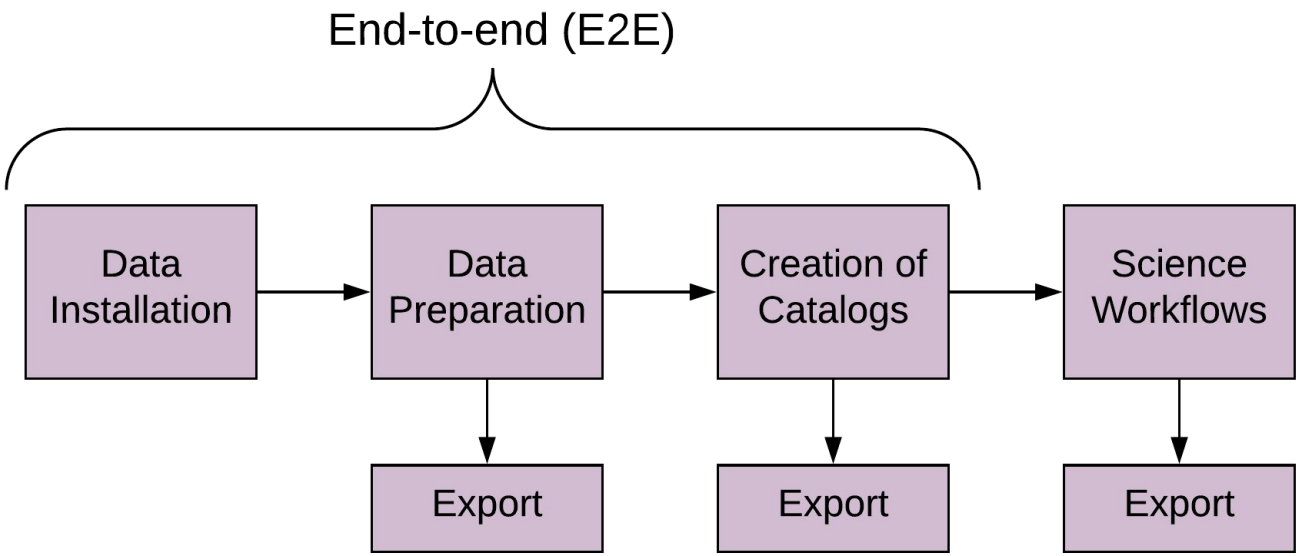
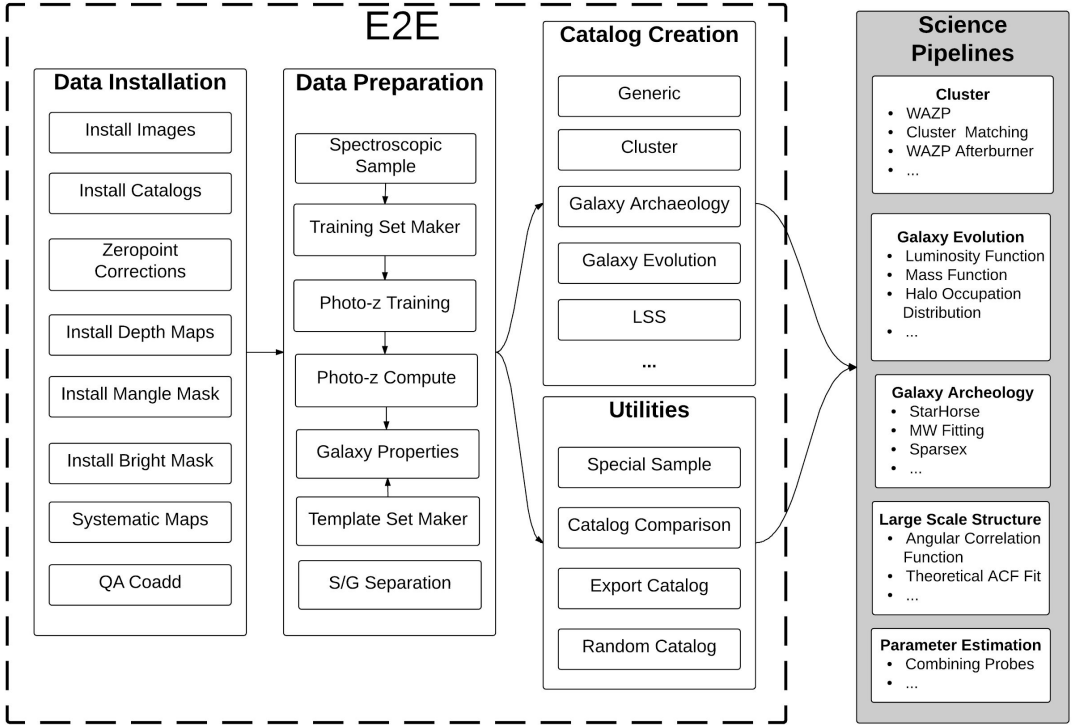


E2E


End-to-end (E2E)
Data Installation
Data Preparation
Creation of Catalogs
Science Workflows
Export
Export
Export

E2E


E2E
Data Installation
Install Images
Install Catalogs
Zeropoint Corrections
Install Depth Maps
Install Mangle Mask
Install Bright Mask
Systematic Maps
QA Coadd
Data Preparation
Spectroscopic Sample
Training Set Maker
Photo-z Training
Photo-z Compute
Galaxy Properties
Template Set Maker
S/G Separation
Catalog Creation
Generic
Cluster
Galaxy Archaeology
Galaxy Evolution
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Utilities
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Science Pipelines
Cluster
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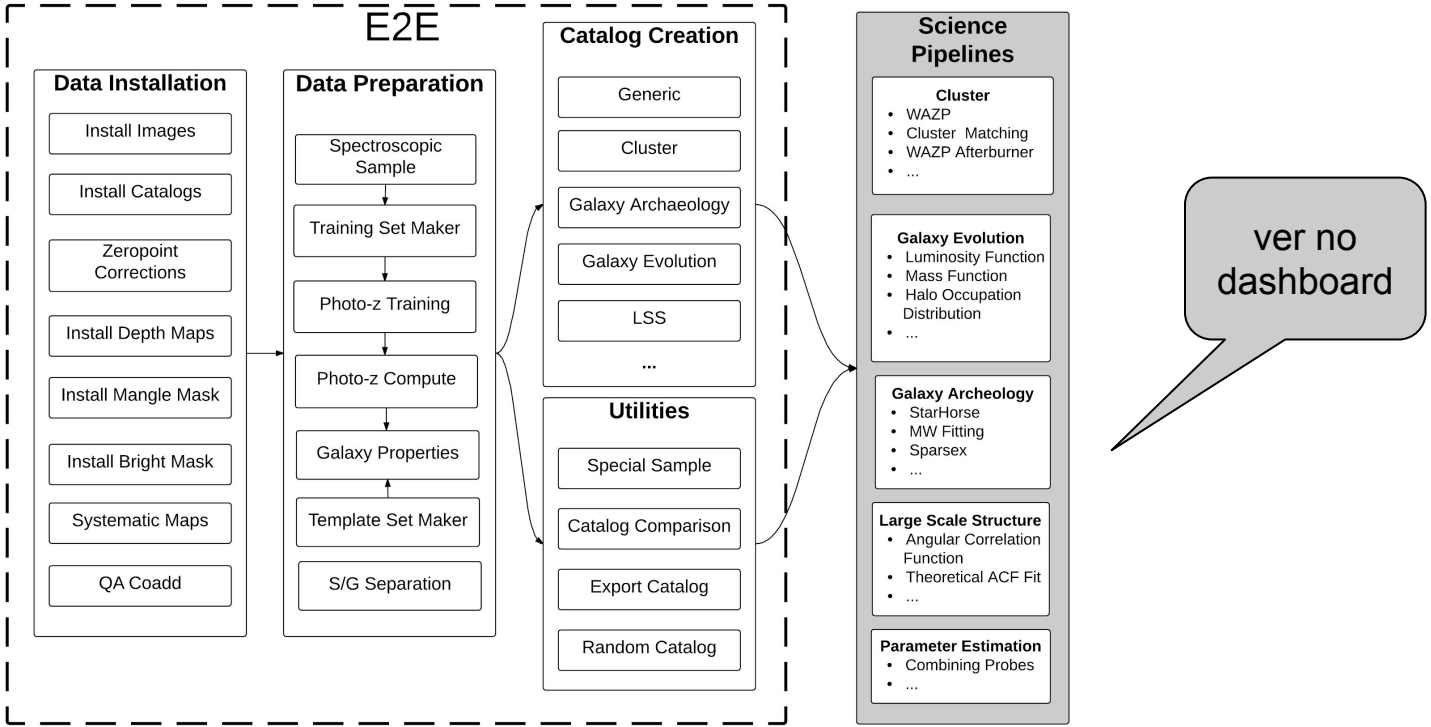
E2E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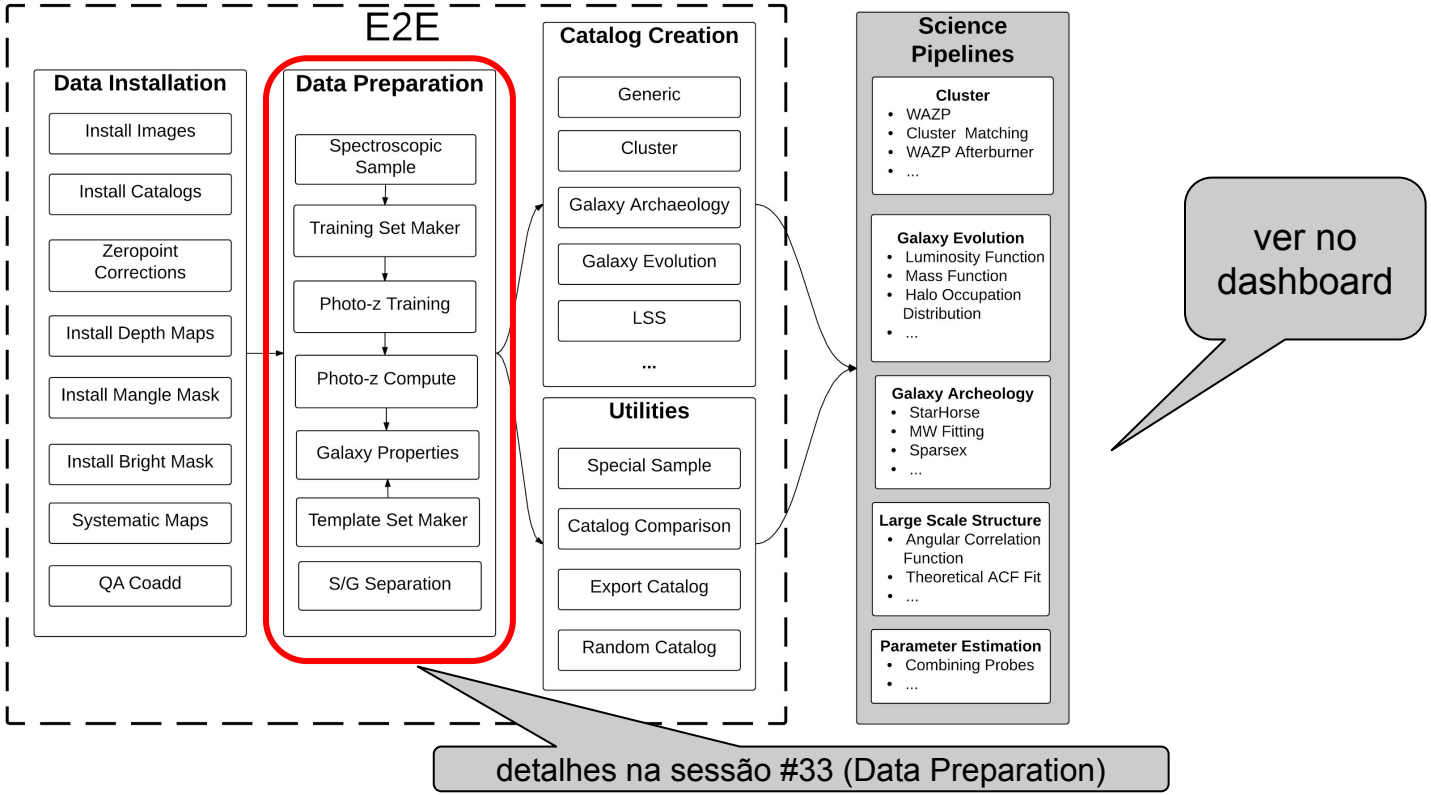
ver no dashboard

E2E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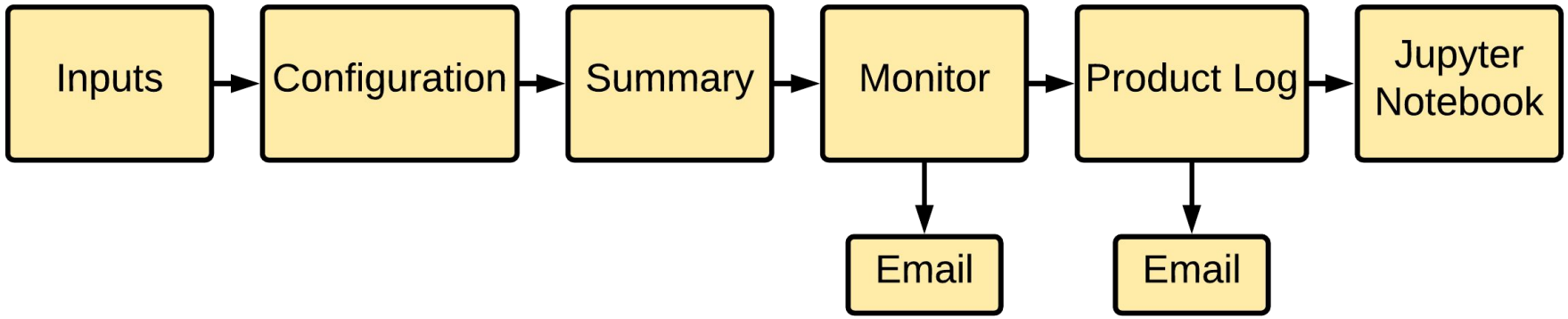
detalhes na sessão #33 (Data Preparation)

Rotina de execução



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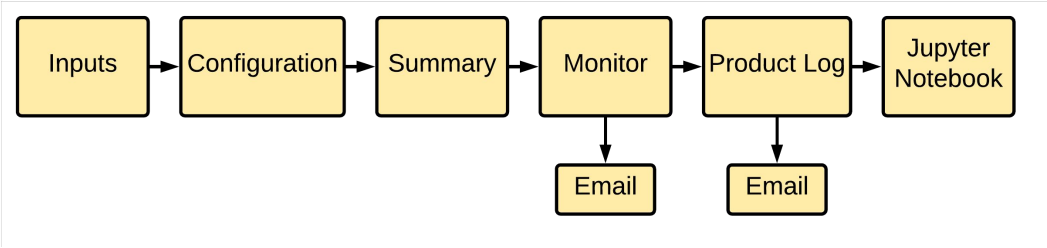

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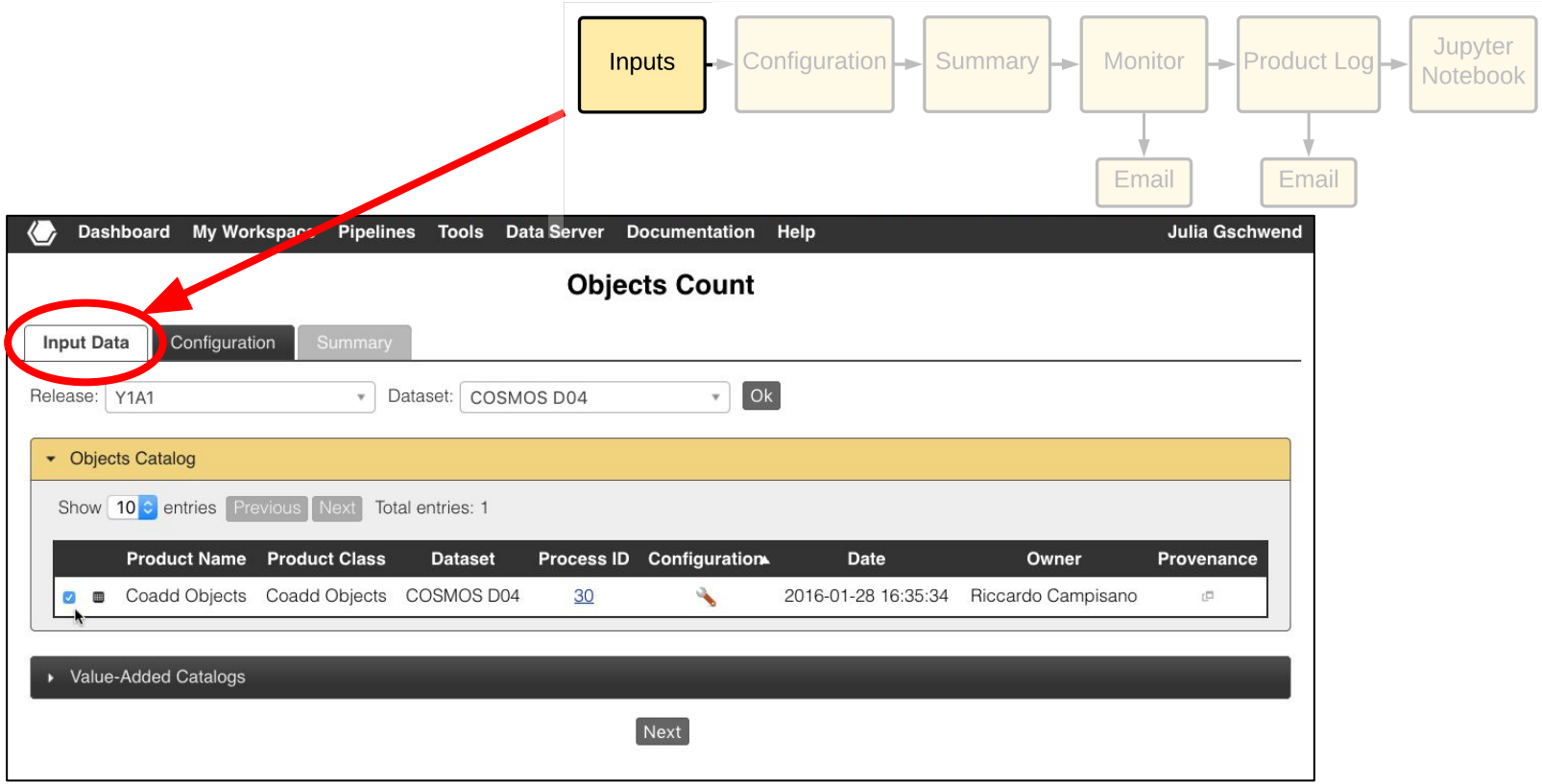

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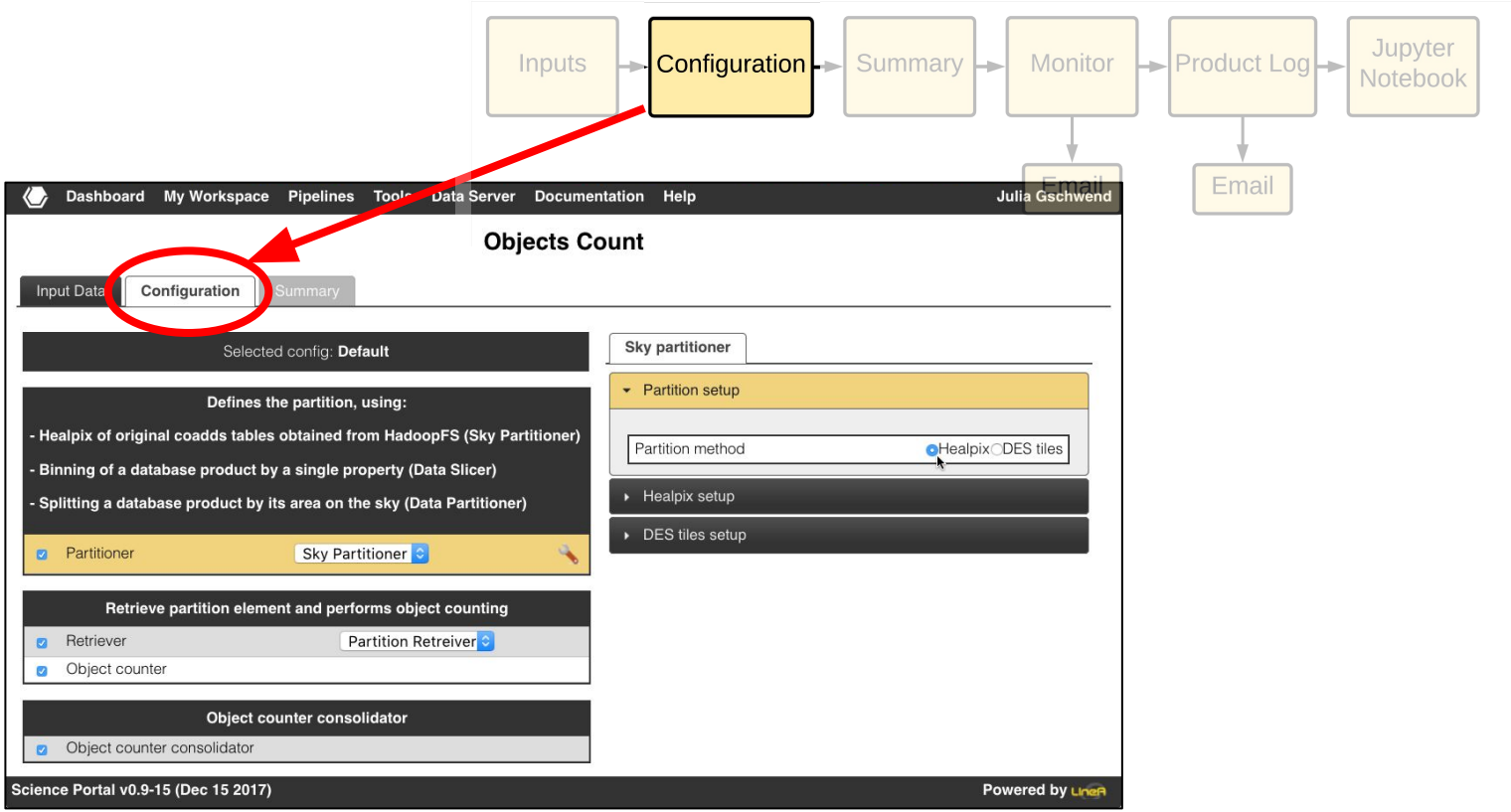

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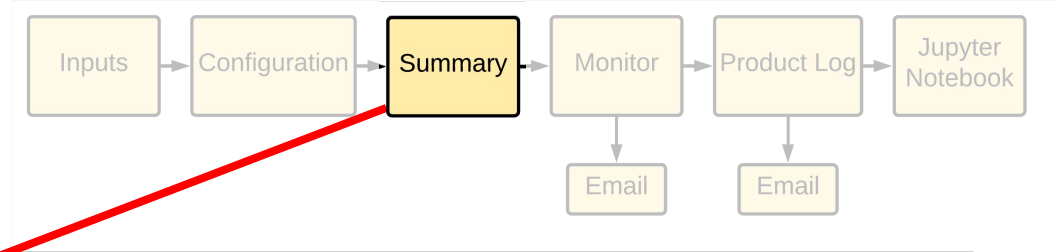

Dashboard | My Workspace | Pipelines | Tools | Data Server | Documentation | Help | Julia Gschwend

Objects Count

Input Data | Configuration | Summary

Input Data

Show 10 entries Previous Next Total entries: 1

	Product Type	Product Name	Product Class	Dataset	Process ID	Configuration	Date	Owner	Provenance
	Objects Catalog	Coadd Objects	Coadd Objects	COSMOS D04	30		2016-01-28 16:35:34	Riccardo Campisano	

Selected Config

Submit

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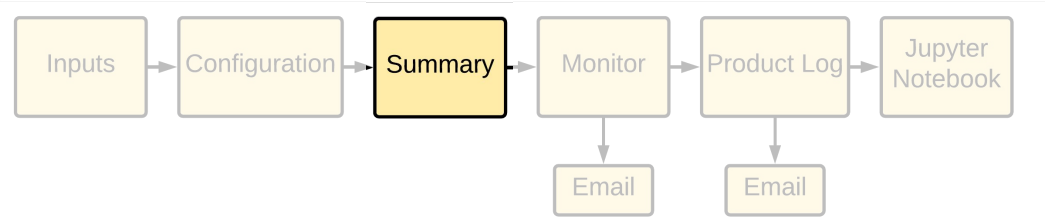

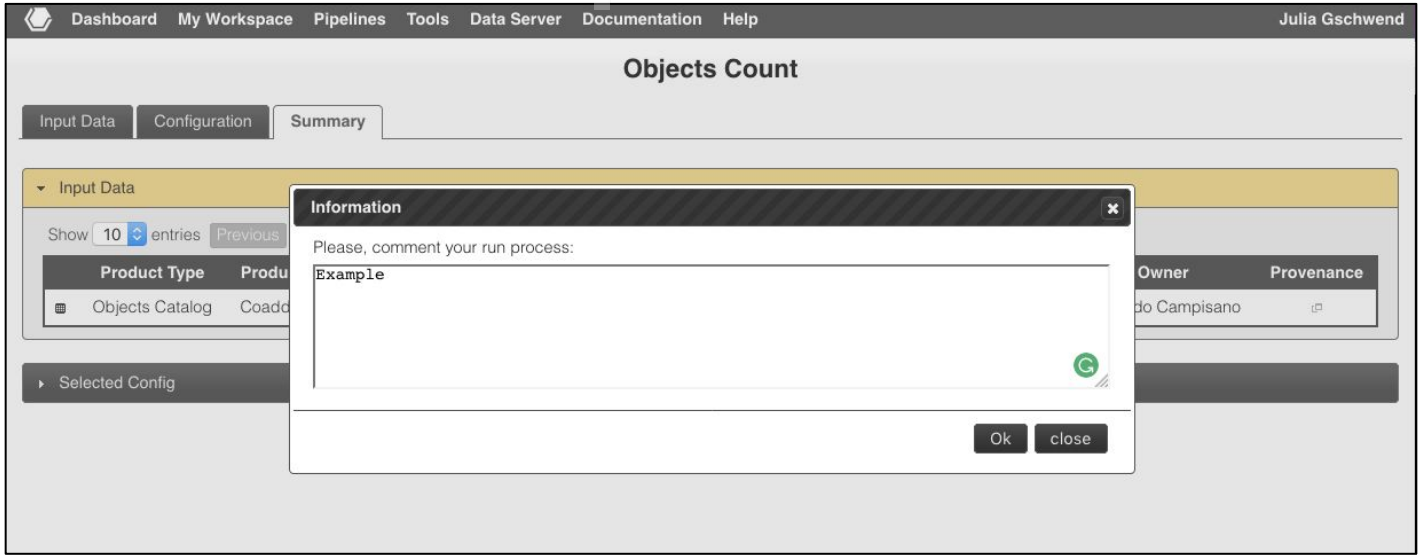

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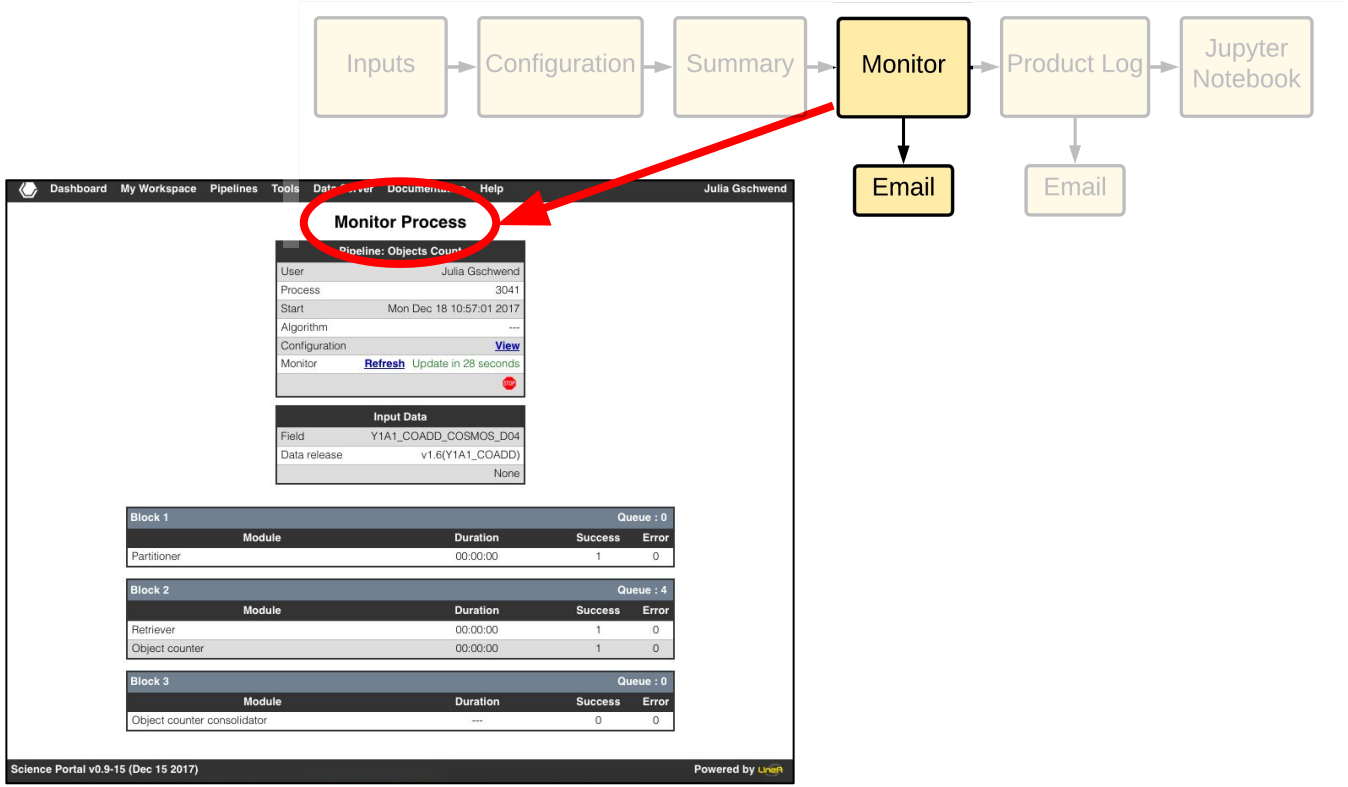

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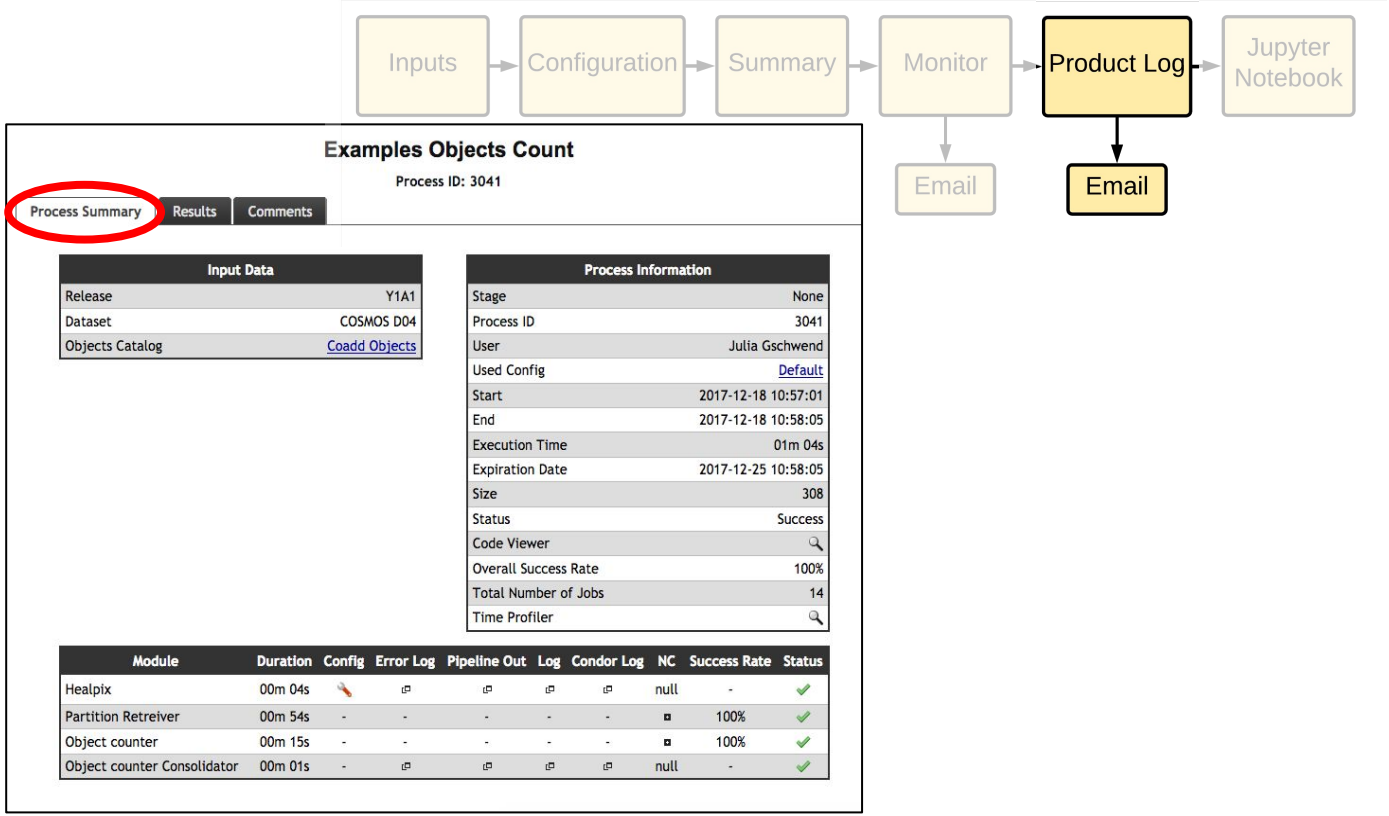

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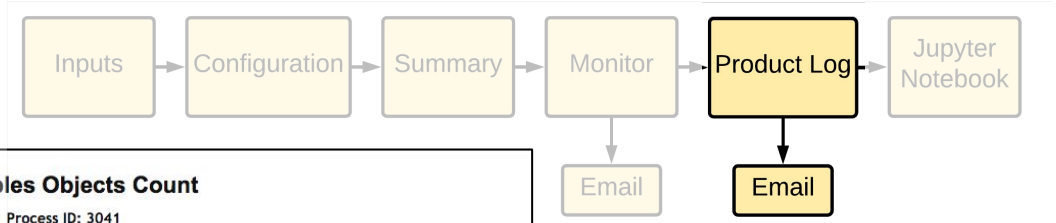

Examples Objects Count

Process ID: 3041

Process Summary | Results | Comments

Summary

Quick Navigation

- Provenance
  - Data Installation
- Total count result
- Count results per file

Provenance

Data Installation

Install Catalogs	30

Total count result

Total objects	313380

Count results per file

6811_cropped_file	43807
6836_cropped_file	16655
6812_cropped_file	2051
6833_cropped_file	256
6814_cropped_file	250589
6809_cropped_file	22

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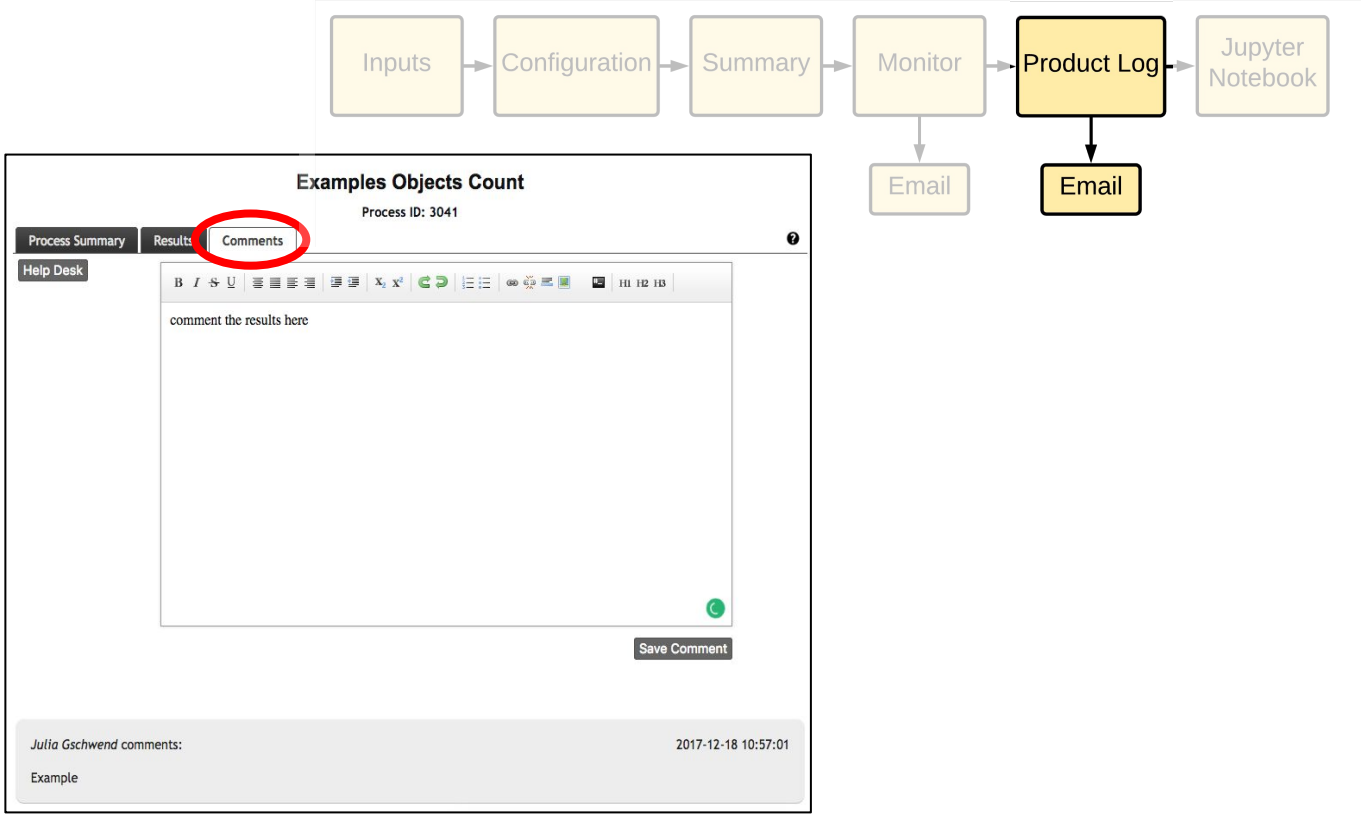


Rotina de execução

jupyter session_14 Last Checkpoint: 6 minutos atrás (unsaved changes)

File Edit View Insert Cell Kernel Widgets Help

In [11]:
```
clean_dataframe = dataframe[mask]
```

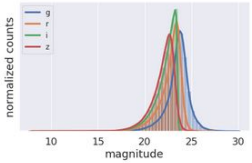
In [12]:
```
clean_dataframe.describe()
```

Out[12]:

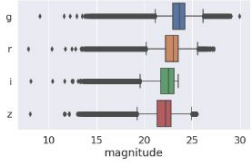
	g	r	i	z
count	368601.000000	368601.000000	368601.000000	368601.000000
mean	23.531657	22.705673	22.198102	21.933851
std	1.248835	1.213079	1.165934	1.215701
min	9.104441	7.882928	8.141896	8.123552
25%	22.992320	22.181051	21.671283	21.352619
50%	23.669358	23.006179	22.520864	22.199848
75%	24.232287	23.518718	23.059547	22.776319
max	29.900811	27.242888	23.500000	25.463392

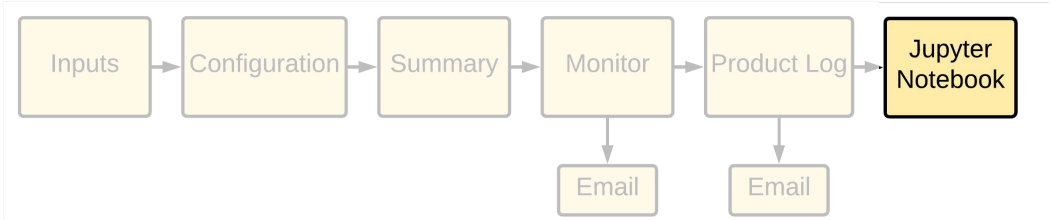
Distribuição de magnitudes

In [13]:
```
sns.distplot(clean_dataframe['g'], hist=True, kde_kws={'label':'g', 'lw':3})
sns.distplot(clean_dataframe['r'], hist=True, kde_kws={'label':'r', 'lw':3})
sns.distplot(clean_dataframe['i'], hist=True, kde_kws={'label':'i', 'lw':3})
sns.distplot(clean_dataframe['z'], hist=True, kde_kws={'label':'z', 'lw':3})
pl.legend(fontsize=12, loc='upper left')
pl.xlabel('magnitude')
pl.ylabel('normalized counts')
pl.yticks([])
pl.tight_layout()
```



In [14]:
```
sns.boxplot(data=clean_dataframe, orient='h')
pl.xlabel('magnitude')
pl.tight_layout()
```





exemplo na sessão #14
(tutorial: criando um Jupyter notebook I)

Lendo uma tabela do banco de dados

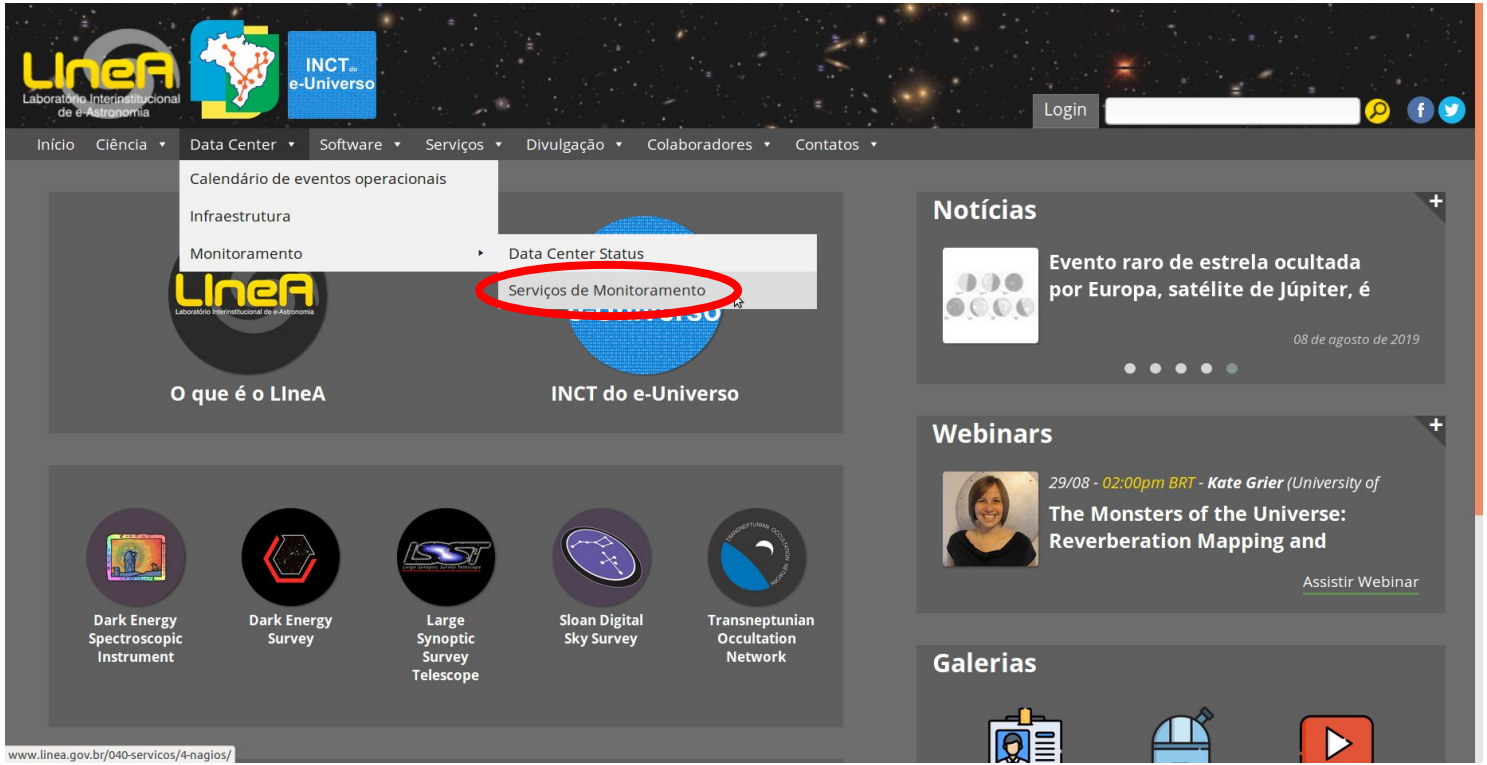
In [2]:
```
tablename = 'vac_ge.catalog_5347'
```

In [3]:
```
engine = sqlalchemy.create_engine('postgres://untrustedprod:untrusted@desdb4.linea.gov.br:5432/prod_gavo')
conn = engine.connect()
```

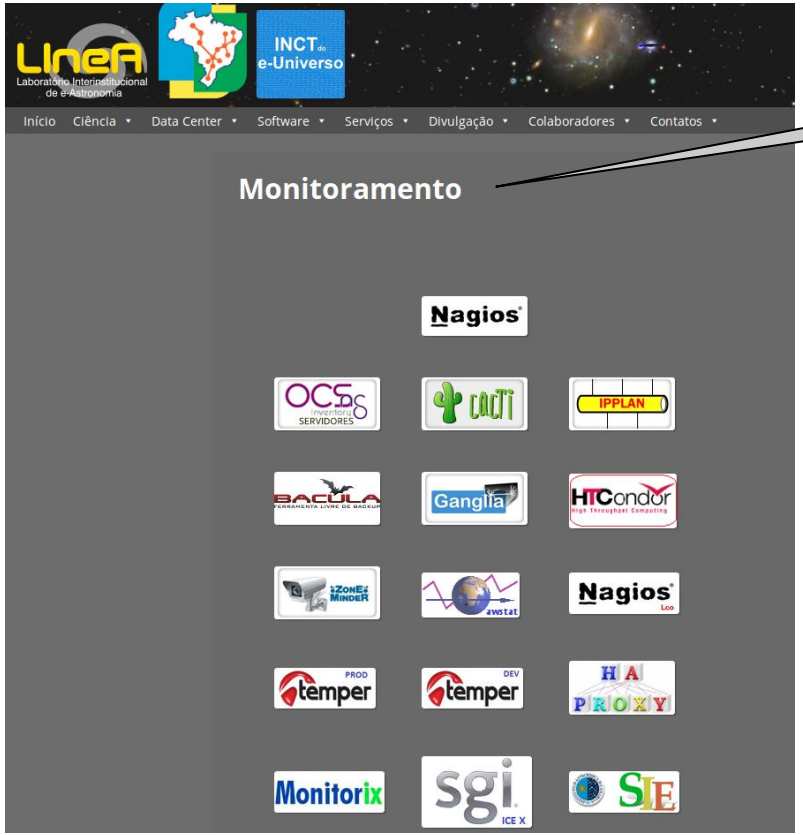
In [4]:
```
#query = 'select mag_g, mag_r, mag_i, mag_z from %s order by random() limit 10000' % tablename
query = 'select mag_g, mag_r, mag_i, mag_z from %s' % tablename
```

In [5]:
```
stm = sqlalchemy.sql.text(query)
stm_get = conn.execute(stm)
stm_result = stm_get.fetchall()
table = Table(rows=stm_result, names=('g', 'r', 'i', 'z'))
dataframe = table.to_pandas()
```

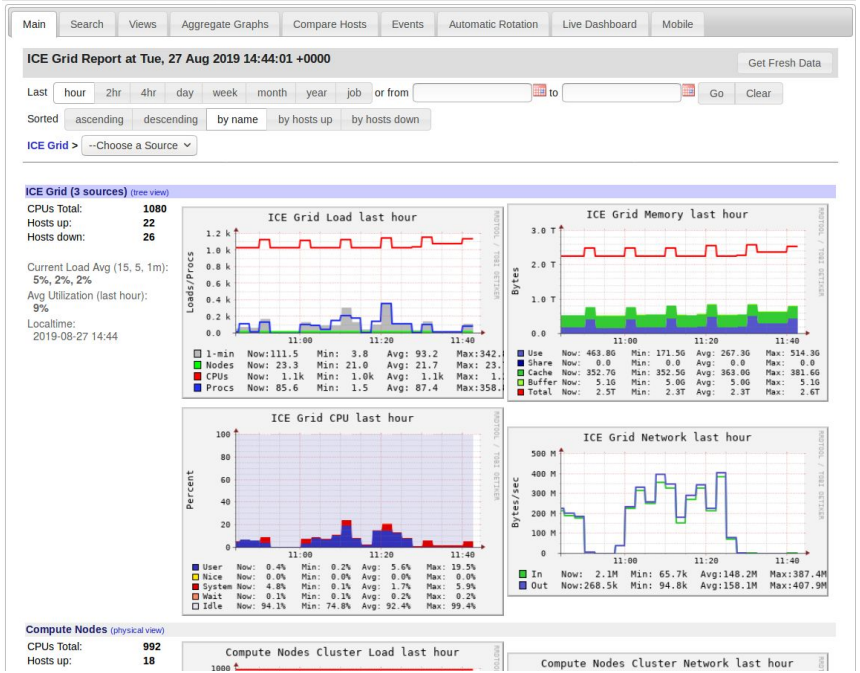
Monitoramento



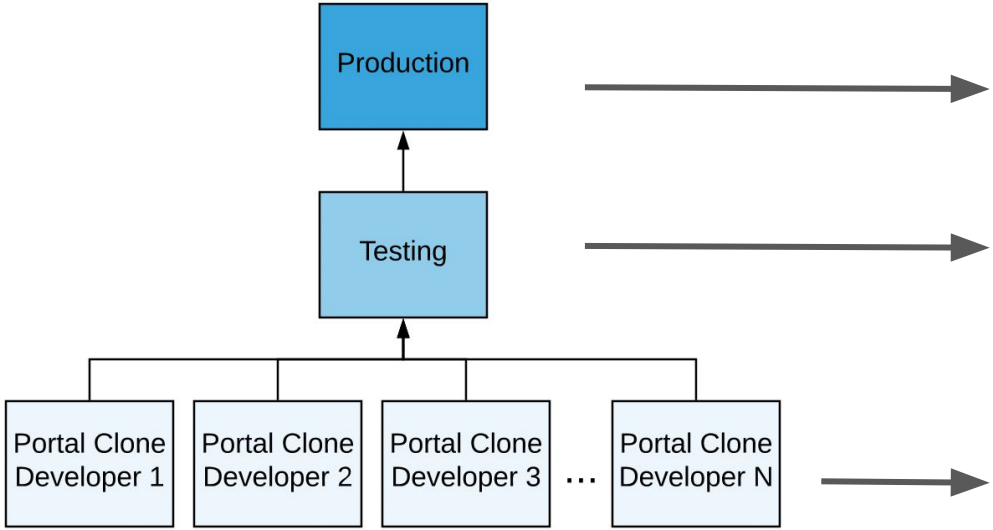
Monitoramento



detalhes na sessão #03



Portal clones - versionamento com GIT



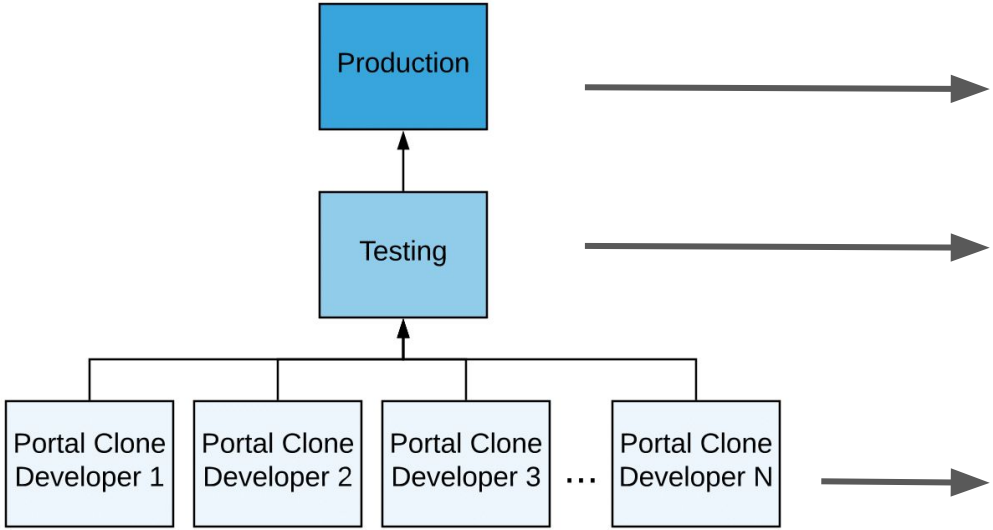
https://des-portal.linea.gov.br/

https://testing.linea.gov.br/

https://julia.linea.gov.br/

Portal clones - versionamento com GIT

Sugestão de tutoriais sobre GIT:
https://learngitbranching.js.org/
https://swcarpentry.github.io/git-novice/



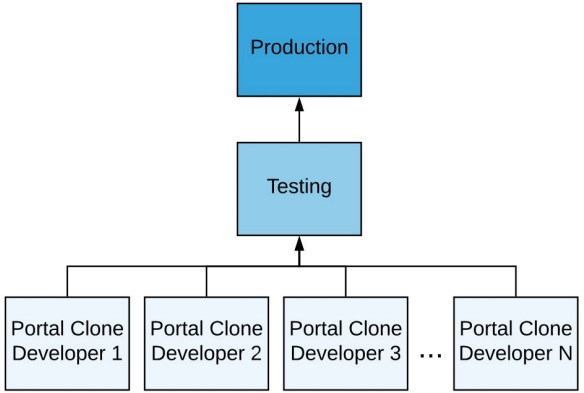
https://des-portal.linea.gov.br/

https://testing.linea.gov.br/

https://julia.linea.gov.br/

Rotina de desenvolvimento

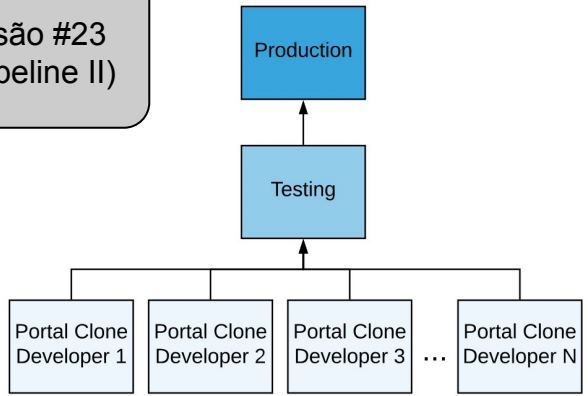
1. Alterar código no seu clone
2. Testar alteração no seu clone
3. Debugar na sandbox, se necessário
4. Versionar mudanças
5. Atualizar Testing
6. Testar a nova versão em Testing
7. Deploy em production
    - Science workflow: atualizar documentação e rodar ferramenta de fast deploy
    - E2E: atualizar documentação e enviar e-mail para CCB



Rotina de desenvolvimento

demonstração na sessão #23
(tutorial: criando um pipeline II)

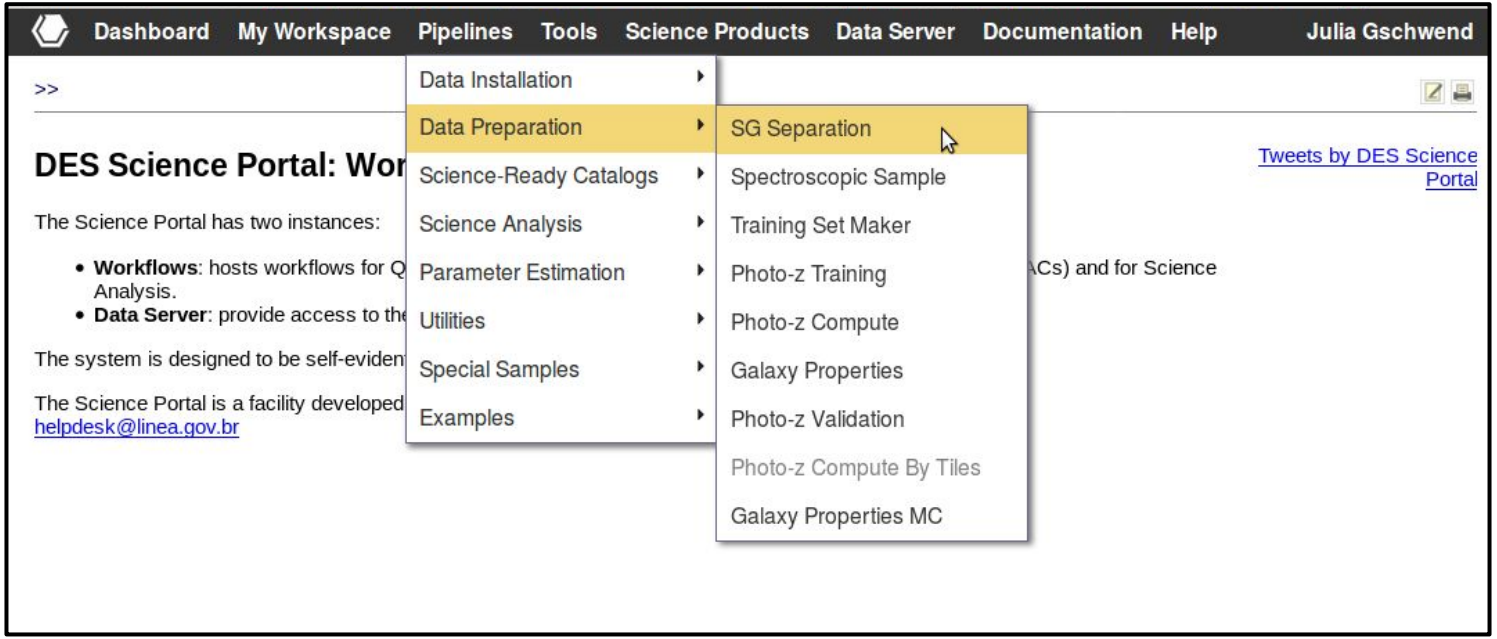
1. Alterar código no seu clone
2. Testar alteração no seu clone
3. Debugar na sandbox, se necessário
4. Versionar mudanças
5. Atualizar Testing
6. Testar a nova versão em Testing
7. Deploy em production
    - Science workflow: atualizar documentação e rodar ferramenta de fast deploy
    - E2E: atualizar documentação e enviar e-mail para CCB



DIY: rodando um pipeline do E2E no portal

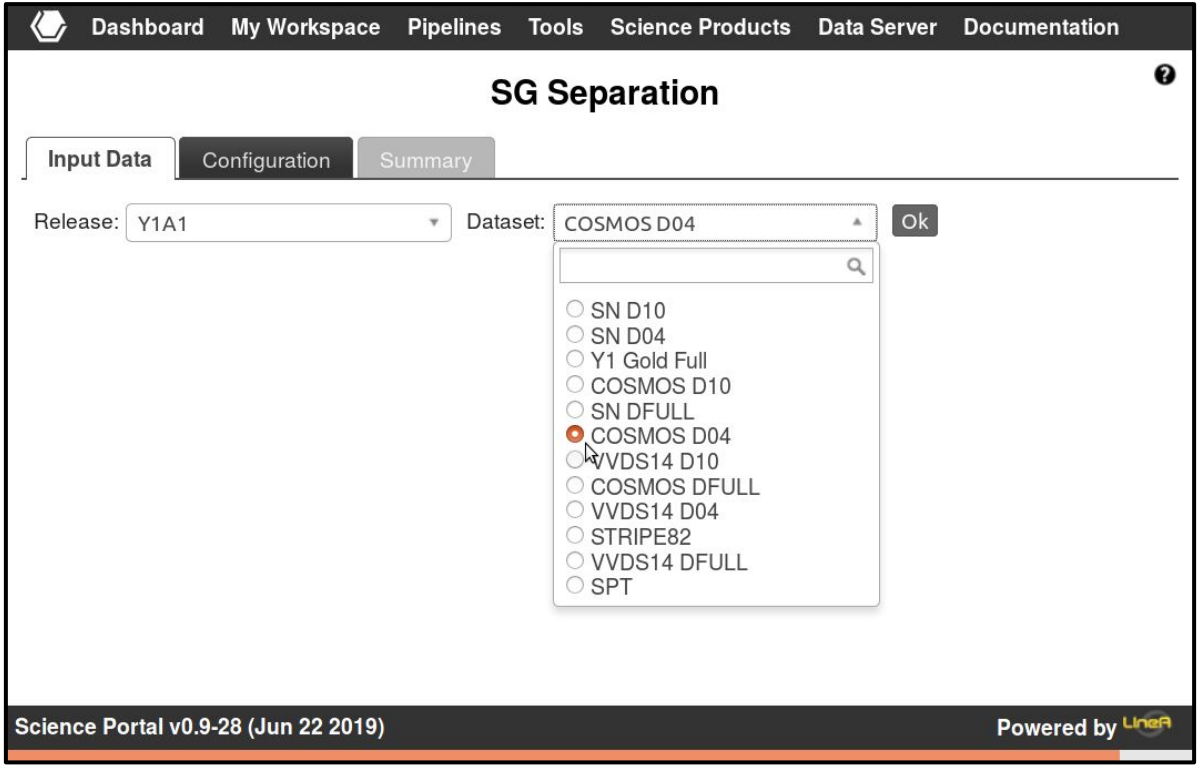
Pipeline Star/Galaxy Separation

https://testing.linea.gov.br/



DIY: rodando um pipeline do E2E no portal

Dados de entrada



DIY: rodando um pipeline do E2E no portal

Dados de entrada

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Release: Y1A1 Dataset: COSMOS D04 Ok

Objects Catalog

Show 10 entries Previous Next Total entries: 1

	Product Name	Product Class	Dataset	Process ID	Configuration	Date	Owner	Provenance
☑	Coadd Objects	Coadd Objects	COSMOS D04	30		2016-01-28 16:35:34	Riccardo Campisano	

Zeropoints

Next

Science Portal v0.9-28 (Jun 22 2019) Powered by LIneA

DIY: rodando um pipeline do E2E no portal

Configurações

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Selected config: **Default**

Data Partitioning
- Data Partitioner

Classification
- Data Retriever
- S/G separation

Consolidator
- Consolidate Results

Configuration
Save | Select | Share with users | Share with groups | Reset | Set as default

Sky partitioner
- Partition setup
  - Partition method: Healpix / DES tiles
- Healpix setup
- DES tiles setup

Science Portal v0.9-28 (Jun 22 2019) — Powered by LIneA

DIY: rodando um pipeline do E2E no portal

Configurações

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Selected config: **Default**

Data Partitioning
- Data Partitioner

Classification
- Data Retriever
- S/G separation

Consolidator
- Consolidate Results

Configuration: Save | Select | Share with users | Share with groups | Reset | Set as default

Sky partitioner
- Partition setup
- Healpix setup
  - Healpix nside: 32
  - Optimize Healpix nside reduction grouping sub-pixels of the same super-pixel in the same job: Yes / No
- DES tiles setup

Next

Science Portal v0.9-28 (Jun 22 2019) — Powered by LIneA

DIY: rodando um pipeline do E2E no portal

Configurações

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Selected config: **Default**

Data Partitioning
- Data Partitioner

Classification
- Data Retriever
- S/G separation

Consolidator
- Consolidate Results

Configuration

Save | Select | Share with users | Share with groups | Reset | Set as default

Setup | Columns

Split Internally

Split data into the exact amount of available processors? Yes No

Minimum chunk size -rows- 100

DIY: rodando um pipeline do E2E no portal

Configurações

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Selected config: **Default**

Data Partitioning
- Data Partitioner

Classification
- Data Retriever
- S/G separation

Consolidator
- Consolidate Results

Configuration: Save | Select | Share with users | Share with groups | Reset | Set as default

General configurations | Specific configurations

Choose classifiers to be executed

CLASS_STAR	True	False
SPREAD_MODEL	True	False
SVA1 MODEST	True	False
Y1 MODEST V1	True	False
Y1 MODEST V2	True	False
Y1 MODEST V3	True	False
Y1 MODEST V4	True	False
Y3 EXTENDED CLASS (SPREAD MODEL)	True	False
Y3 EXTENDED CLASS (WAVG SPREAD MODEL)	True	False

- Photometric corrections
- General parameters for SVA1
- General parameters for Y1A1

Science Portal v0.9-28 (Jun 22 2019) | Powered by LIneA

DIY: rodando um pipeline do E2E no portal

Resumo

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Input Data

Show 10 entries Previous Next Total entries: 1

	Product Type	Product Name	Product Class	Dataset	Process ID	Configuration	Date	Owner	Provenance
	Objects Catalog	Coadd Objects	Coadd Objects	COSMOS D04	30		2016-01-28 16:35:34	Riccardo Campisano	

Selected Config

Submit

DIY: rodando um pipeline do E2E no portal

Comentário de submissão

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

SG Separation

Input Data | Configuration | Summary

Input Data

Show 10 entries | Previous | Next | Total entries: 1

Product Type	Product Name	Product Class	Dataset	Process ID	Configuration	Date	Owner	Provenance
Objects Catalog	Coadd O						ardo Campisano	

Selected Config

Information

Please, comment your run process:

exemplo bootcamp

Ok | close

Monitoramento

Dashboard | My Workspace | Pipelines | Tools | Science Products | Data Server | Documentation | Help | Julia Gschwend

Monitor Process

Pipeline: SG Separation	
User	Julia Gschwend
Process	5559
Start	Mon Aug 26 17:23:49 2019
Algorithm	---
Configuration	View
Monitor	Refresh Update in 23 seconds

Input Data	
Field	Y1A1_COADD_COSMOS_D04
Data release	v1.6(Y1A1_COADD)
	Data Preparation

Block 1 — Queue : 0

Module	Duration	Success	Error
Data Partitioner	00:00:00	1	0

Block 2 — Queue : 5

Module	Duration	Success	Error
Data Retriever	00:00:00	1	0
S/G separation	00:00:00	1	0

Block 3 — Queue : 0

Module	Duration	Success	Error
Consolidate Results	---	0	0

Science Portal v0.9-28 (Jun 22 2019) — Powered by LineA

Product Log

Data Preparation SG Separation

Process ID: 10035102

Process Summary | Results | Comments

Input Data	
Release	Y1A1
Dataset	COSMOS D04
Objects Catalog	Coadd Objects

Additional Information	
Y1 modest v4	Yes
# of galaxies	272371
# of stars	41009
Fraction of sources analyzed	1.00

Process Information	
Stage	Data Preparation
Process ID	10035102
User	Julia Gschwend
Used Config	Default
Start	2019-08-27 09:29:34
End	2019-08-27 09:32:45
Execution Time	03m 11s
Expiration Date	2019-09-03 09:32:45
Size	496184
Status	Success
Code Viewer	
Overall Success Rate	100%
Total Number of Jobs	14
Time Profiler	

Output Data	
S/G Classification	Y1 Modest v4 11

Module	Duration	Config	Error Log	Pipeline Out	Log	Condor Log	NC	Success Rate	Status
Sky Partitioner	0:00:03						nc53	-	
Partition Retreiver	0:00:48		-	-	-	-		100%	
Star Galaxy Separation	0:00:48		-	-	-	-		100%	
Consolidate Results	0:01:35	-					nc53	-	

Data Preparation SG Separation

Process ID: 10035102

Process Summary | Results | Comments

Summary | Y1 Modest v4

Quick Navigation
Provenance
Data Installation
Sky partitioner
Number of files

Provenance

Data Installation

Install Catalogs	10024396

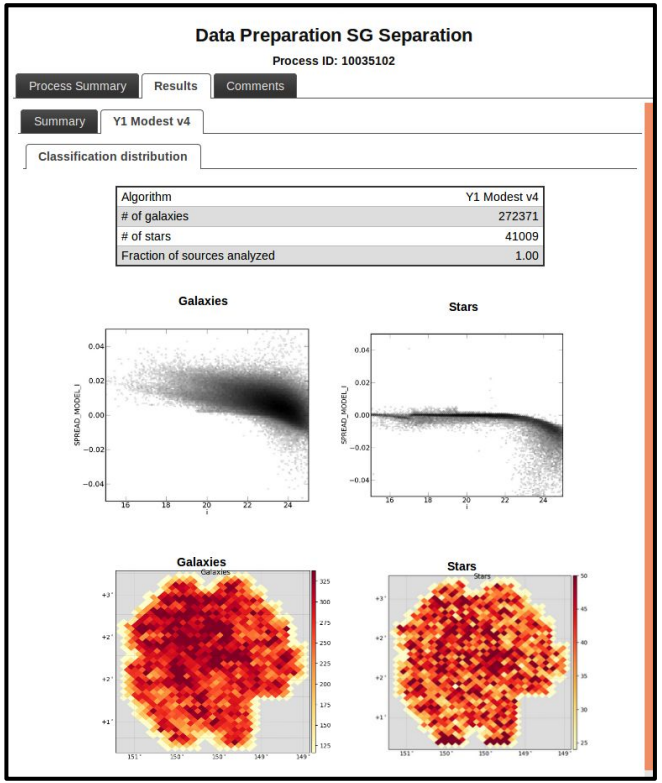
Sky partitioner

Input NSIDE	32
Output NSIDE	32
Number of threads	6

Number of files

Y1 Modest v4	95

Product Log

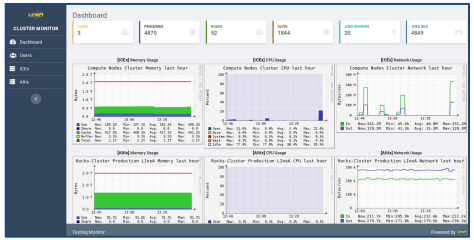

Data Preparation SG Separation
Process ID: 10035102
Process Summary
Results
Comments
Summary
Y1 Modest v4
Classification distribution
Algorithm Y1 Modest v4
# of galaxies 272371
# of stars 41009
Fraction of sources analyzed 1.00
Galaxies
Stars
SPREAD_MODEL_i
i
Galaxies
Stars

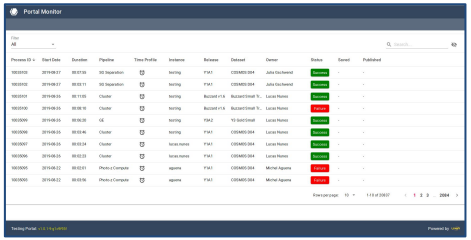
Data Preparation SG Separation
Process ID: 10035102
Process Summary
Results
Comments
Help Desk
Save Comment
Julia Gschwend comments:
2019-08-27 09:29:34
product log for bootcamp slides

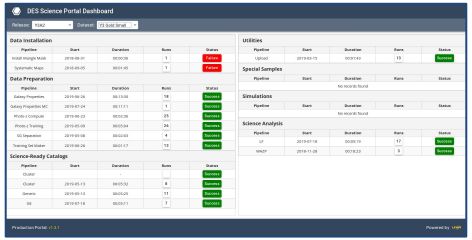
O futuro do portal

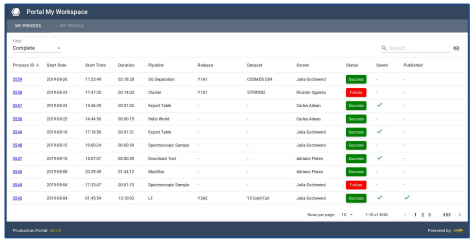
DES Science Portal (“Portal 1.0”)

- DES Y6
- modernização → separação em micro-serviços





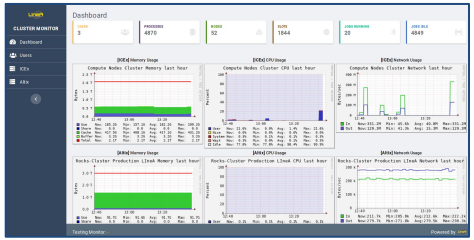


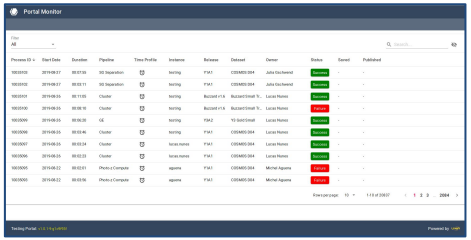


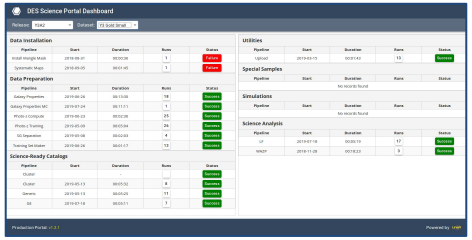
O futuro do portal

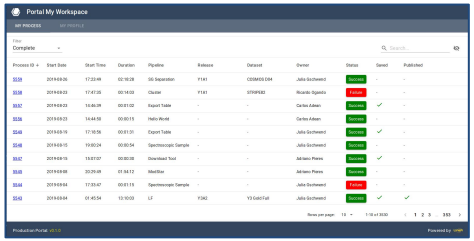
DES Science Portal (“Portal 1.0”)

- DES Y6
- modernização → separação em micro-serviços









novo Science Portal (“Portal 2.0”)

- em fase de idealização e design
- nova tecnologia
- lições aprendidas com o DES Science Portal (1.0)

detalhes na sessão #24

Dúvidas?

Sessão 20 - Portal científico: Introdução

Calendário do Bootcamp

	2	3	4	5	6
9:00 - 9:30	**1- Introdução ao LIneA** L. Nicolaci - 45'	**9- Introdução ao LIneA II** L. Nicolaci - 45'	**17- Usando o Santos Dumont** V. Lima - 30'	**Colaborações Científicas** **25- DES** - B. Santiago - 25' **26- DESI** - F. Oliveira - 25' **27- SDSS** - J. Schimoia - 25' **28- TON** - J. Camargo - 25'	**37- Documentação** C.Silveira - 30'
9:30 - 10:00	**2- LIneA: Como se registrar** G. Soares - 30'	**10- Trabalhando no LIneA** A. Nunes - 45'	**18- Usando o Santos Dumont: Casos de Uso** H. Camacho, A. Pieres - 30'		**38-Transferência de Dados** J. Souza - 20' **39- Máquinas Virtuais, Containers e Kubernetes** J. Souza - 20'
10:00 - 10:30	**Coffee break** 15'		**Foto e Coffee break** 30'		**40- Rede Nacional de Ocultação** G. Rossi - 30'
10:30 - 11:00	**3- LIneA: Infraestrutura** C. Adean - 45'	**Coffee break** 15' **11- Ferramentas Colaborativas** F. Massena - 30'	**19- Uso Avançado da Infraestrutura** C. Adean - 45'	**Coffee break** 20' (inicio 10:40)	**Coffee break** 20' (inicio 10:40)
11:00 - 11:30	**4- Landing Page do LIneA** C. Silveira - 30'	**12- Ferramentas Astronômicas I** C. Singulani - 30'	**20- Portal Cientifico: Introdução** J.Gschwend - 45'	**Colaborações Científicas** **29- LSST** - L. Nicolaci - 30'	**41- Ciberinfraestrutura para Apoio à e-Ciência** A. Moura - 30'
11:30 - 12:00				**30- Atividades Científicas** A. Pieres - 30'	**42- Atividades de EPO** E. Nogueira - 30'
12:00 - 12:30	**Almoço** 75'	**Almoço** 75'	**Almoço** 60'	**Almoço** 60'	**Almoço** 60'
12:30 - 13:00					
13:00 - 13:30	**5- Spotlight talks** R. Boufleur - 90'	**13- Ferramentas Astronômicas II** G. Costa - 60'	**21- Criando um Pipeline no Portal I** C. Singulani, L. Nunes - 60'	**31- Analisando DES Y6** R. Gruendl - 60´	**43- Planejando o Futuro** A. Nunes, A. Pieres - 150'
13:30 - 14:00					
14:00 - 14:30		**14- Jupyter Notebooks: Criando** J.Gschwend - 30'	**22- Portal Científico: Workflows Científicos** A. Pieres, M. Aguena - 45'	**32- DES - Primary Products** A. Pieres - 45´	
14:30 - 15:00	**6- Serviços** F. Massena - 30'	**15- Jupyter Notebooks: Usando e Desenvolvendo** A. Pieres, M. Aguena - 60'	**23- Criando um Pipeline no Portal II** J.Gschwend - 60'	**33- DES Portal - Data Preparation** J.Gschwend - 45´	
15:00 - 15:30	**7- Jupyter Notebooks: Introdução** G. Soares - 30'				
15:30 - 16:00	**Coffee break** 30'	**Coffee break** 30'	**Coffee break** 30'	**Coffee break** 30'	**44- Perspectivas do LIneA** L. Nicolaci - 30'
16:00 - 16:30	**8- Jupyter Notebooks: Exemplos** A. Pieres - 60'	**16- Jupyter Notebooks: Casos de Uso** F. Oliveira, R. Boufleur - 60'	**24- Requisitos para o Portal do LSST** M.Sanchez - 45'	**34- Validando Imagens DES Y6** A. Pieres - 30´	**Encerramento** 30'
16:30 - 17:00				**35- Validando Catálogos DES Y6** M. Aguena - 30´	**Legenda** Apresentação Tutorial Hacksession/Hands on
17:00 - 17:30	**Q&A** 30'	**Q&A** 30'	**Q&A** 30'	**36- Explorando Dados DES Y6** M. Aguena - 30´	