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Centro Nazionale di Ricerca in HPC,  
Big Data and Quantum Computing



Centro Nazionale di Ricerca in HPC,  
Big Data and Quantum Computing

# Integrating Universal Immune System Simulator in a Cloud, GDPR compliant, environment

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Incontro Plenario Spoke 8, Casalecchio di Reno (BO) 25/06/2024

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# *Outline*

- Requirements
- Technical Implementation
- Current status & future works
- References
- Acknowledgment

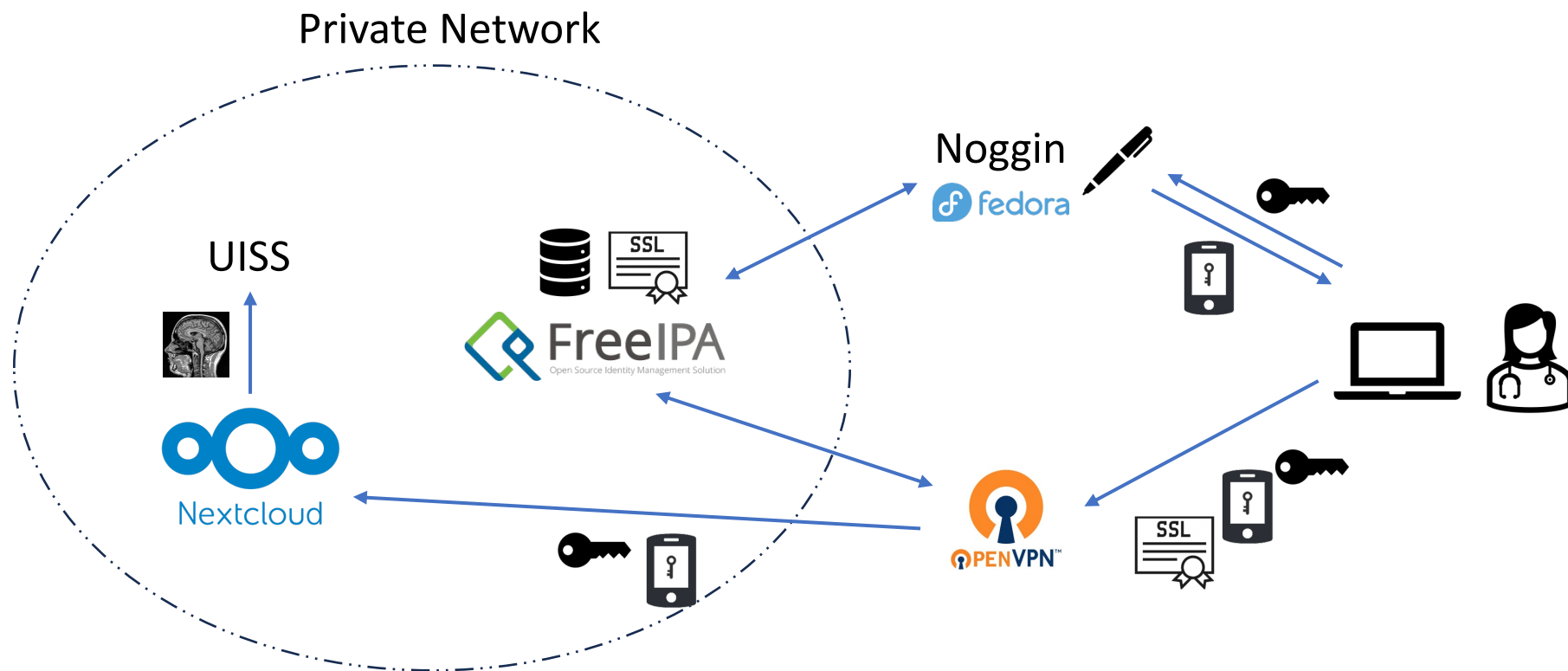
# *Universal Immune System Simulator*

- Use medical data
- Simulate & predict immune system response
- Model disease progression
- Find best therapy according immune system profiles

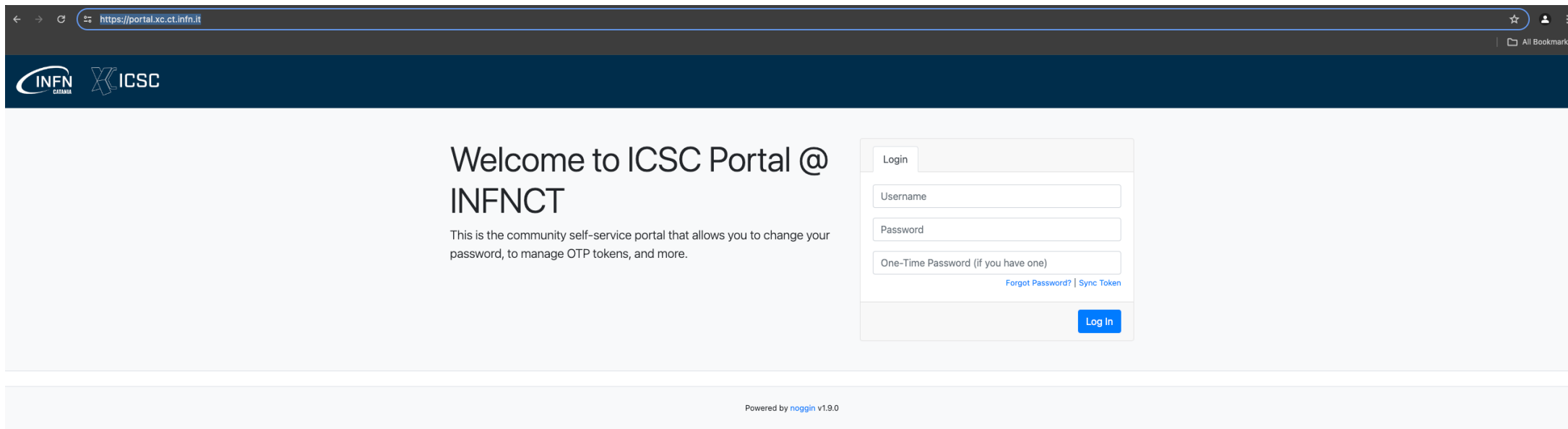
# Requirements

- **Data security**
  - ISO 9001 – 27001 Certified Server
  - Data managed according GDPR regulation
  - Restricted access to identified users
- **Network security**
  - Application secured by VPN
  - Two factor authentication
- **User Friendly**
- **Scalability**

## Technical Implementaion



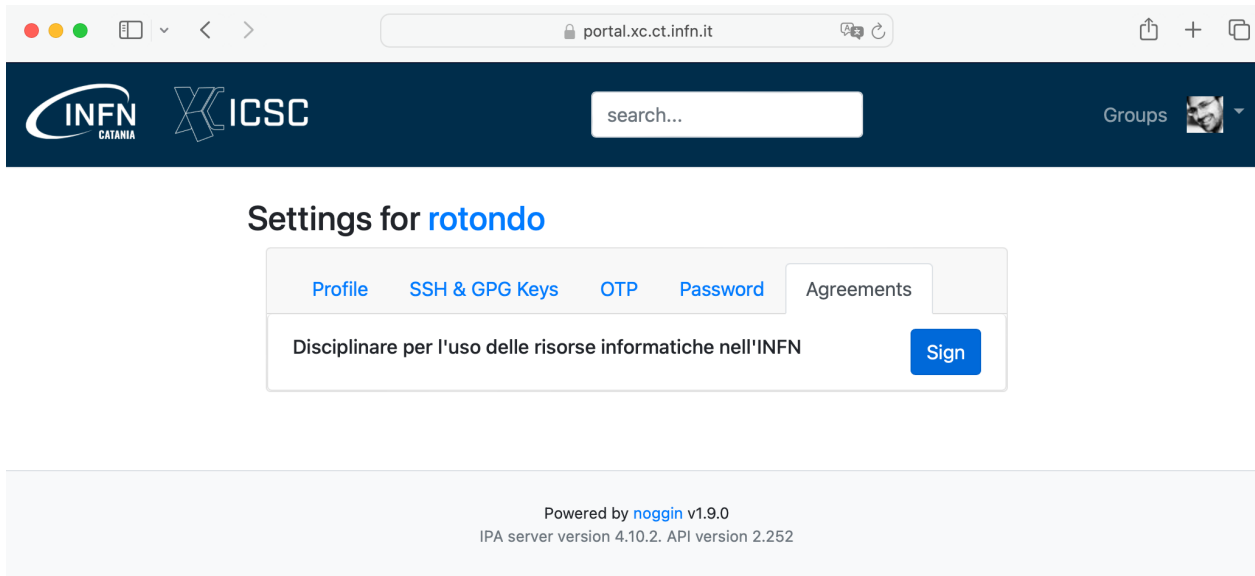
# *Technical Implementation*



The screenshot shows a web browser window with the URL <https://portal.xc.ct.infn.it>. The page header features the INFN and ICSC logos. The main content area displays a welcome message: "Welcome to ICSC Portal @ INFNCT" followed by a brief description: "This is the community self-service portal that allows you to change your password, to manage OTP tokens, and more." To the right is a login form with fields for "Login", "Username", "Password", and "One-Time Password (if you have one)". Below the last field are links for "Forgot Password?" and "Sync Token". A blue "Log In" button is positioned at the bottom right of the form. At the bottom of the page, it says "Powered by noggin v1.9.0".

■ <https://portal.xc.ct.infn.it>

# Tecnical Implementation



portal.xc.ct.infn.it

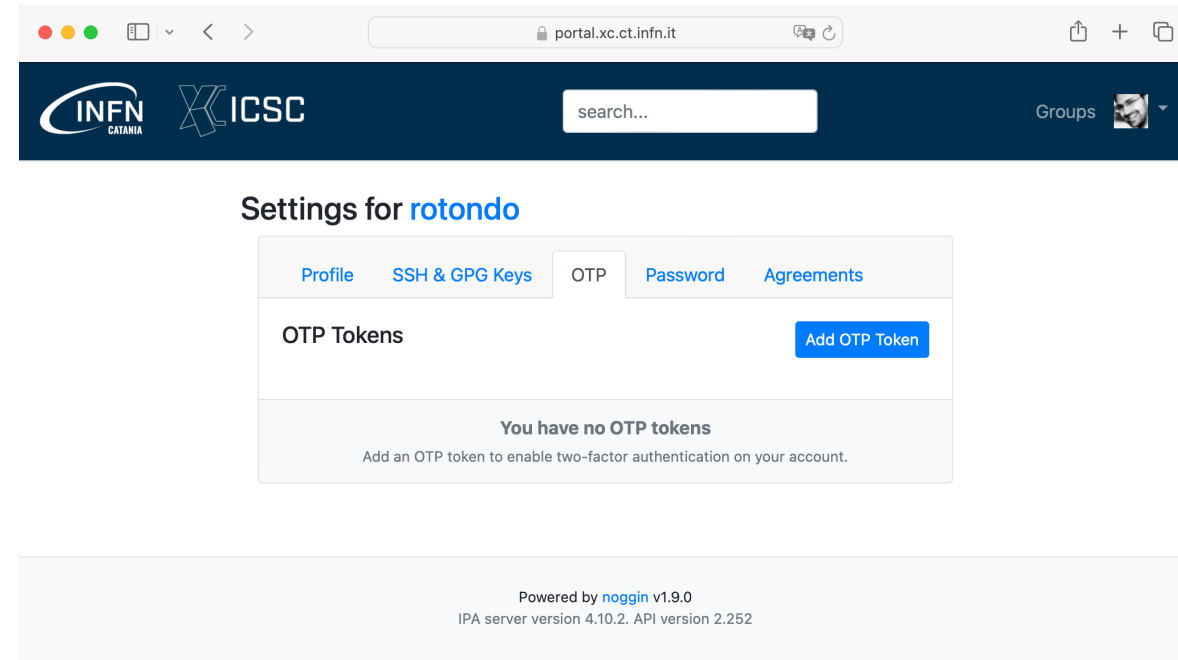
INFN CATANIA ICSC search... Groups

### Settings for rotondo

Profile SSH & GPG Keys OTP Password Agreements

Disciplinare per l'uso delle risorse informatiche nell'INFN [Sign](#)

Powered by [noggin](#) v1.9.0  
IPA server version 4.10.2. API version 2.252



portal.xc.ct.infn.it

INFN CATANIA ICSC search... Groups

### Settings for rotondo

Profile SSH & GPG Keys OTP Password Agreements

OTP Tokens [Add OTP Token](#)

**You have no OTP tokens**  
Add an OTP token to enable two-factor authentication on your account.

Powered by [noggin](#) v1.9.0  
IPA server version 4.10.2. API version 2.252

■ <https://portal.xc.ct.infn.it>

## Tecnical Implementation

**ICSC**  
Centro Nazionale di Ricerca in HPC,  
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**INFN**  
CATANIA

Username

Password

[Log In Using Certificate](#) [Sync OTP Token](#) [Log in](#)

- To log in with **username and password**, enter them in the corresponding fields, then click 'Log in'.
- To log in with **Kerberos**, please make sure you have valid tickets (obtainable via kinit) and **configured** the browser correctly, then click 'Log in'.
- To log in with **certificate**, please make sure you have valid personal certificate.

■ Freeipa internal server



# Tecnical Implementation

The screenshot shows the INFN CATANIA Identity Management console. The top navigation bar includes 'Identity', 'Policy', 'Authentication', 'Network Services', and 'IPA Server'. The main menu has 'Users', 'Hosts', 'Services', 'Groups', 'ID Views', 'Automember', 'Subordinate IDs', and 'User Agreement'. The 'Active users' section is highlighted, showing a table with columns: User login, First name, Last name, Status, UID, Email address, Telephone Number, and Job Title. Below this, the 'User Agreements' section is shown, featuring a table with columns: Agreement name, Status, and Agreement Description. A single agreement is listed: 'Disciplinare per l'uso delle risorse informatiche nell'INFN' with a status of 'Enabled'.

The screenshot shows the INFN CATANIA Identity Management console with the 'User Groups' section selected. The main menu is the same as in the previous screenshot. The 'User Groups' section displays 'User Group: uiss'. Below this, there are sections for 'uiss members:' and 'uiss is a member of:'. The 'uiss is a member of:' section shows a table with columns: User Groups, Netgroups, Roles, HBAC Rules, Sudo Rules, and User Agreements (1). A single agreement is listed: 'Disciplinare per l'uso delle risorse informatiche nell'INFN'. The bottom of the page shows 'Showing 1 to 1 of 1 entries.'

Freeipa internal server

# USER INTERFACE



- LDAP integration
- Workflow
- UISS-MS OUTPUT

# LDAP integration -Server

LDAP/AD integration - A x +

uiss.xc.ct.infn.it:8443/nextcloud/index.php/settings/admin/ldap

INFN

Personal

- Personal info
- Security
- Notifications
- Sharing
- Appearance and accessibility
- Availability
- Flow
- Privacy
- App order

Administration

- Overview
- Basic settings
- Sharing
- Security
- LDAP/AD integration

### LDAP/AD integration

Server Users Login Attributes Groups Advanced Expert

1. Server: freeipa.xc.infnct +

freeipa.xc.infnct 389 Detect Port

uid=nextclouduser,cn=users,cn=accounts,dc=xc,dc=infnct

..... Save Credentials

dc=xc,dc=infnct Detect Base DN Test Base DN

Manually enter LDAP filters (recommended for large directories)

Configuration OK ● Continue Help

# LDAP integration - Users

`(&(|(objectclass=inetorgperson))(|(memberof=cn=uiss,cn=groups,cn=accounts,dc=xc,dc=infnc)))`

LDAP/AD integration - A x +

uiss.xc.ct.infn.it:8443/nextcloud/index.php/settings/admin/ldap

INFN

Personal

- Personal info
- Security
- Notifications
- Sharing
- Appearance and accessibility
- Availability
- Flow
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- App order

Administration

- Overview
- Basic settings
- Sharing
- Security
- LDAP/AD integration

### LDAP/AD integration

Server **Users** Login Attributes Groups Advanced Expert

Listing and searching for users is constrained by these criteria:

Only these object classes:

The most common object classes for users are organizationalPerson, person, user, and inetOrgPerson. If you are not sure which object class to select, please consult your directory admin.

Only from these groups:

>

<

[Edit LDAP Query](#)

`(&(|(objectclass=inetorgperson))(|(memberof=cn=uiss,cn=groups,cn=accounts,dc=xc,dc=infnc)))`

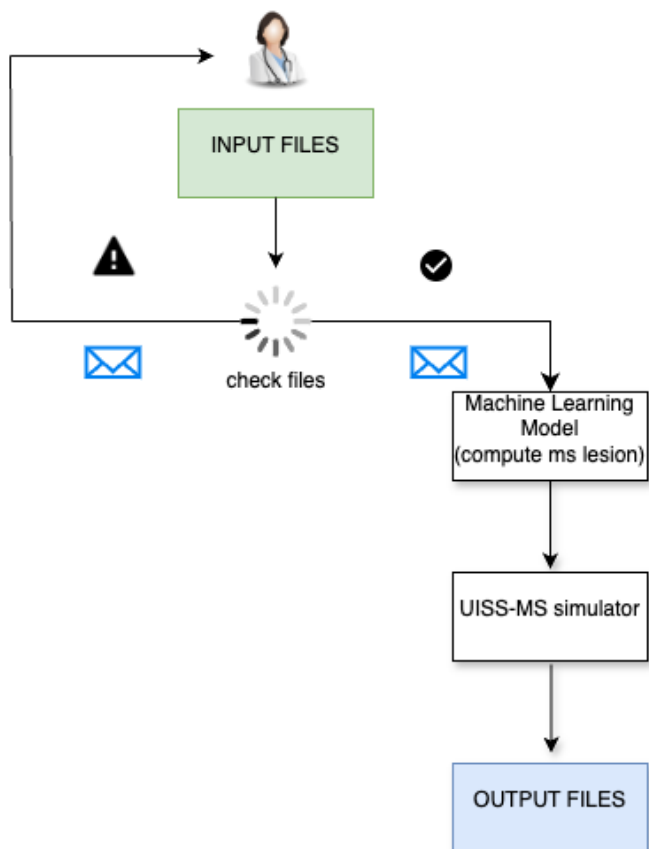
[Verify settings and count users](#)

# LDAP integration - Advanced

The screenshot displays the Windows Settings application interface for LDAP/AD integration. The left sidebar shows the 'Personal' section with options like Personal info, Security, Notifications, Sharing, Appearance and accessibility, Availability, Flow, Privacy, and App order. The main content area is titled 'LDAP/AD integration' and has tabs for 'Server', 'Users', 'Login Attributes', and 'Groups'. The 'Advanced' tab is selected, showing the following settings:

- Connection Settings**
- Directory Settings**
  - User Display Name Field:
  - 2nd User Display Name Field:
  - Base User Tree:
  - User Search Attributes:
  - Disable users missing from LDAP:
  - Group Display Name Field:

# WORKFLOW



```
source $UISS_LESION_VENV_PPATH/bin/activate
pushd $UISS_COMPUTE_MSLV
python compute_ms_lesion_volume.py --root_dir $TEMP_DIR_PY_ROOT --out_dir $TEMP_DIR_PY_OUT --log_dir "/var/log/ui
ss/$username" |& tee /var/log/uiss/$username/$username-$(date +%Y-%m-%d_%H%M%S)-compute-ms-lesion.log
popd

# run simulation in a temporary directory
TEMP_DIR=$(mktemp -p /tmp -d uiss.XXXXXX)

echo "Executing uiss on $filename in ${TEMP_DIR} as working directory"
pushd $TEMP_DIR &> /dev/null
uiss -m "$TEMP_DIR_PY_OUT/output.txt" -f "$TEMP_DIR_PY_OUT/datafile" &> ./run.out

# generating plots
echo "Generating plots"
gnuplot -p /usr/local/share/uiss/script/wrapper.gp

# moving files .out to out directory
mkdir out
mv *.out ./out

# Generating archive result zip file as follows:
# <inputfilename with _ as spaces>-results-<unix timestamp>.zip

ofilename="${filename// /_}-results-$(date +%s).zip"
ofilepath="/var/www/html/nextcloud/data/$username/files/OUTPUT/$ofilename"
echo "Creating archive results file $ofilename"
zip -r "$ofilepath" ./
chown www-data:www-data $ofilepath
sleep 2
```

106,0-1 93%

## Aim



### Longitudinal brain MRI study

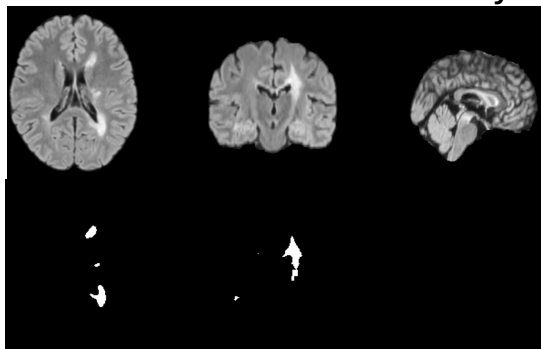
- Automatically segment multiple sclerosis lesions using advanced deep learning techniques
- Compute lesion volume

## Retrospective Dataset



### MSValid Data Collection:

- 75 patients
- Multimodal MRI
- Multiple time-point
- Acquired at different centers
- Masks annotated using the Jim9 Software and validate by doctors.

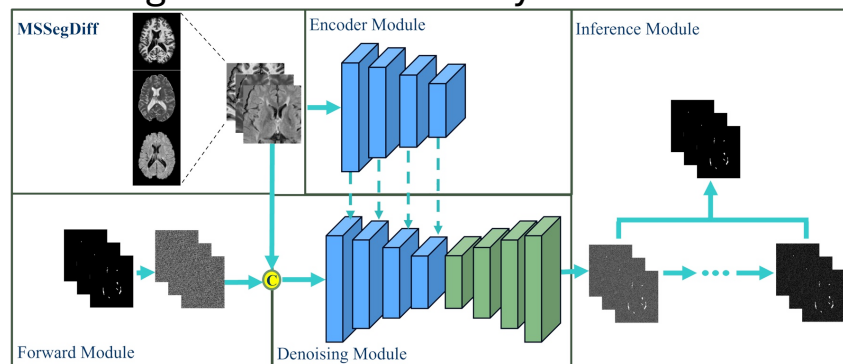


# Compute MS Lesion Volume

## Model



- **Preprocessing:** Anonymization and registration to a 1mm isotropic MNI template
- **Diffusion Model:** Class of generative model, adapted to perform semantic segmentation
- **U-net architecture:** Suitable for medical image segmentation
- **Attention mechanism:** Allows focusing on important image regions, improving segmentation accuracy

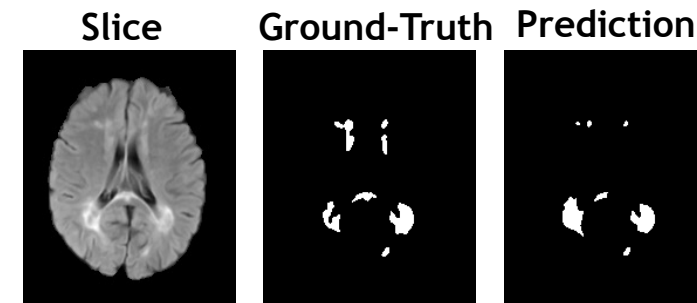


## Model performance



### Evaluation metric:

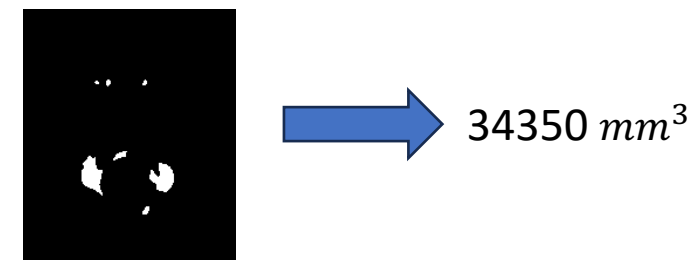
**Dice score:** measure the similarity between two classes



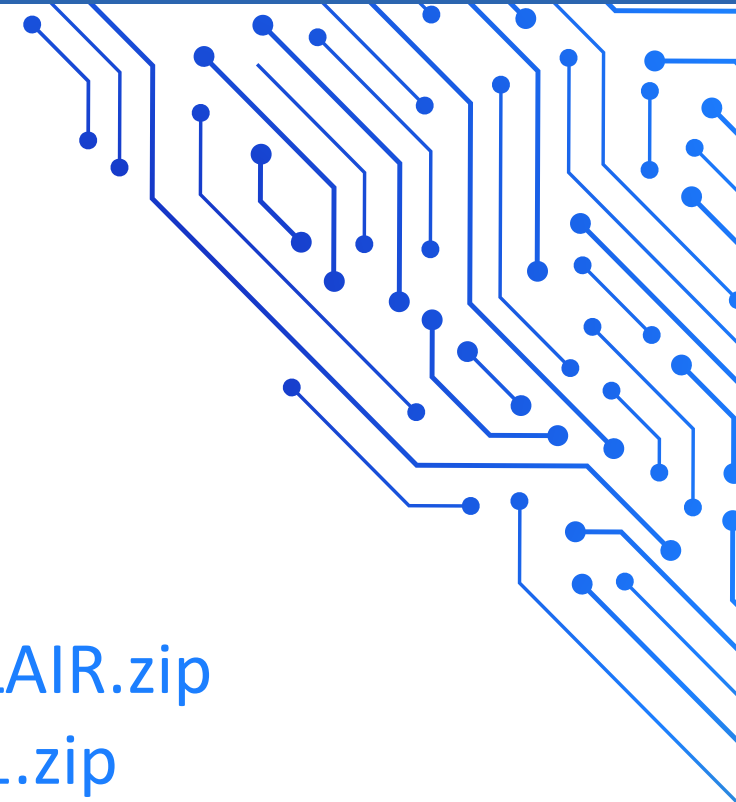
## Compute lesion volume



Volume in  $mm^3$  of the prediction



## RUN UISS simulator - INPUT



FLAIR.zip

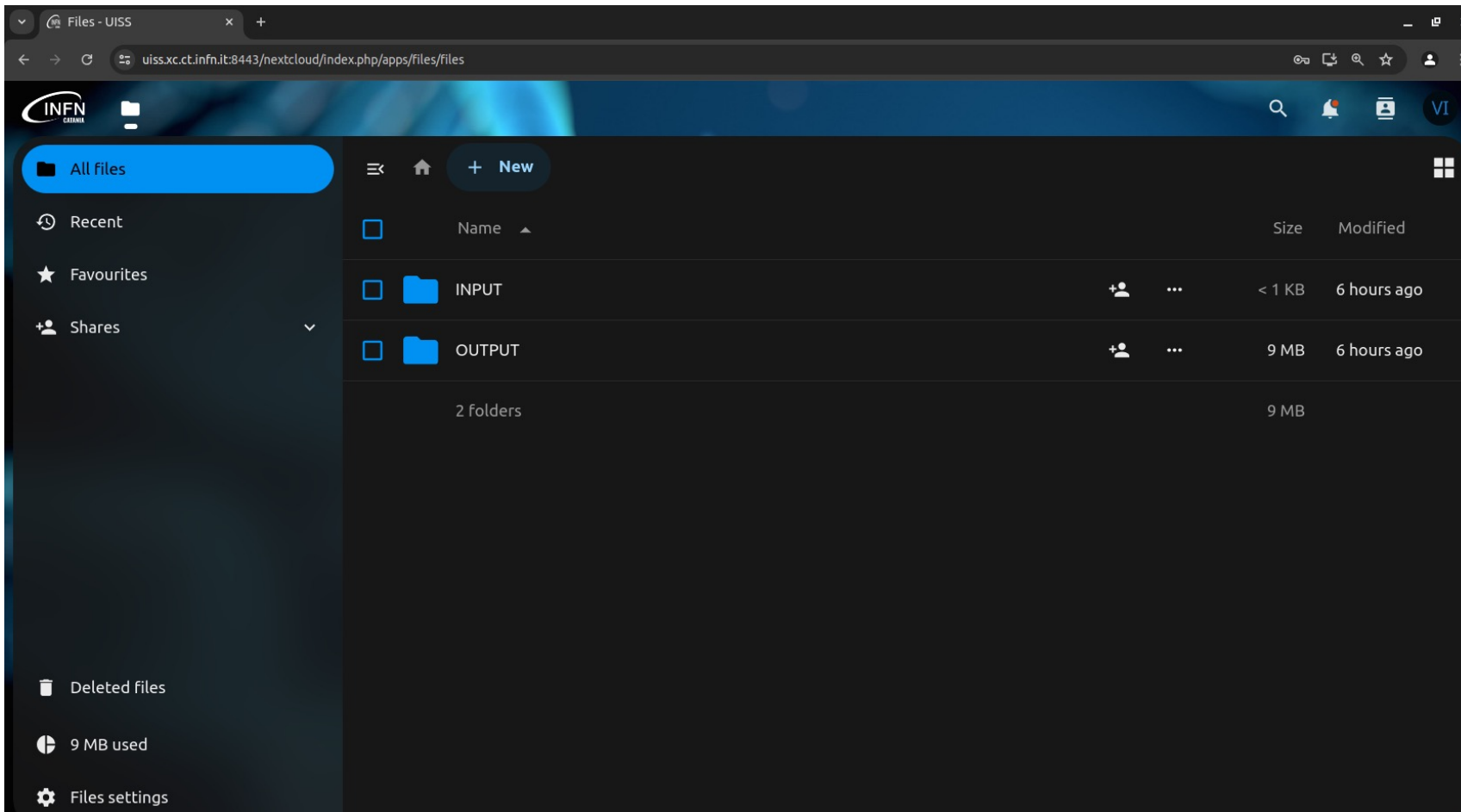
T1.zip

T2.zip

datafile



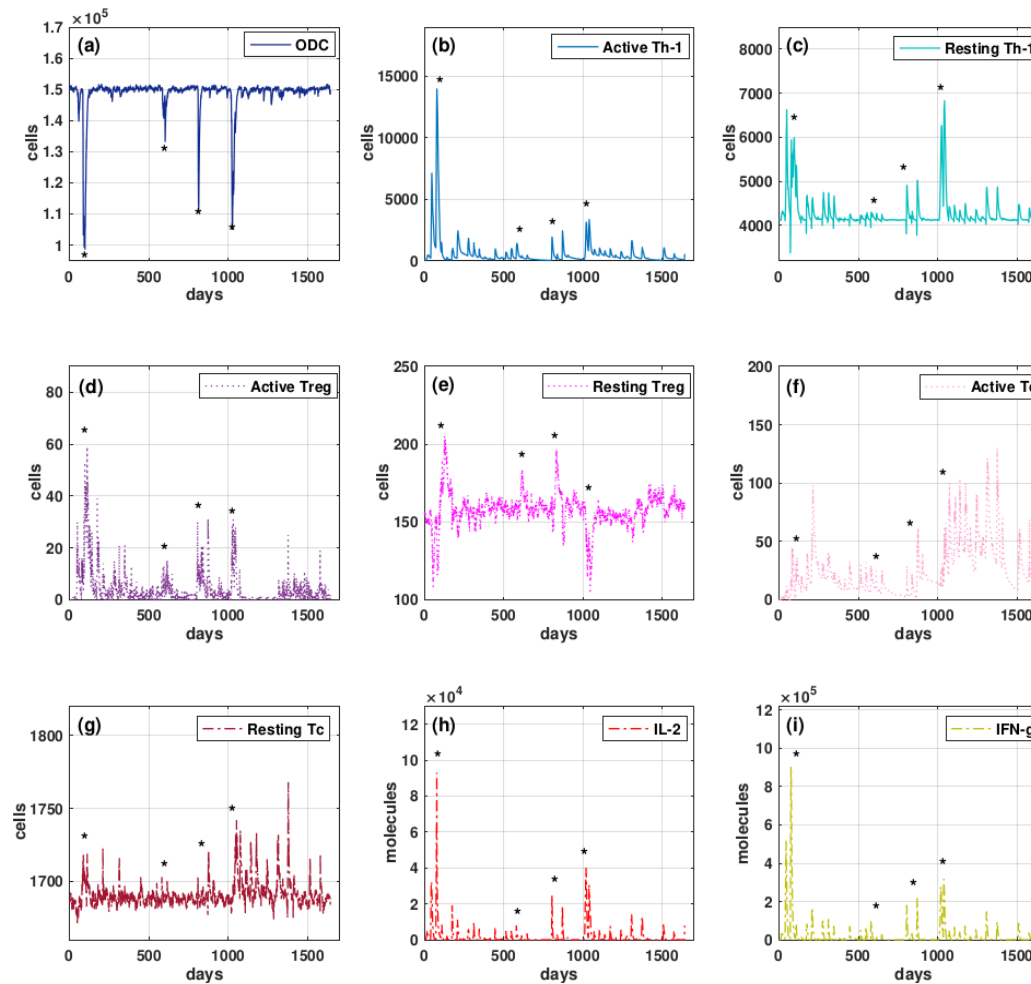
input.zip





# UISS-MS OUTPUT

Predicted cellular and cytokine dynamics



## Current Status & future works

Service	Server	Docker Image	What for INFN Cloud
Noggin	Python VirtualEnv	Available on test branch	Test docker image
Freeipa	Virtual	Custom INFN Image created	Ready
VPN	Virtual	Not available	Prepare docker image or VM
Nextcloud	Physical	Available	Test docker image
UISS	Physical	Not Available	Prepare docker image or VM

## References

- INFN Portal: <https://portal.xc.ct.infn.it>
- Noggin: <https://noggin-aaa.readthedocs.io/en/latest/>
- Freeipa: <https://www.freeipa.org>
- Freeipa INFN container:  
<https://baltig.infn.it/infncct/icsc/spoke8/freeipa-container>
- OpenVPN: <https://openvpn.net>
- Nextcloud: <https://nextcloud.com>
- CQI CERTIQUALITY: <https://www.ct.infn.it/it/servizi-locali/servizio-calcolo-e-reti.html>

# *Acknowledgment*

- Francesco Guarnera<sup>2</sup>
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- Barbara Martelli<sup>1</sup>
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- Alessia Rondinella<sup>2</sup>
- Alessia Tricomi<sup>1,2</sup>

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2. University of Catania



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