Inserm

La science pour la santé
From science to health

OpenDose on EGI: producing reference dosimetric data for Nuclear Medicine on the European Grid Infrastructure

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OpenGate meeting, December 13th 2018, Orsay

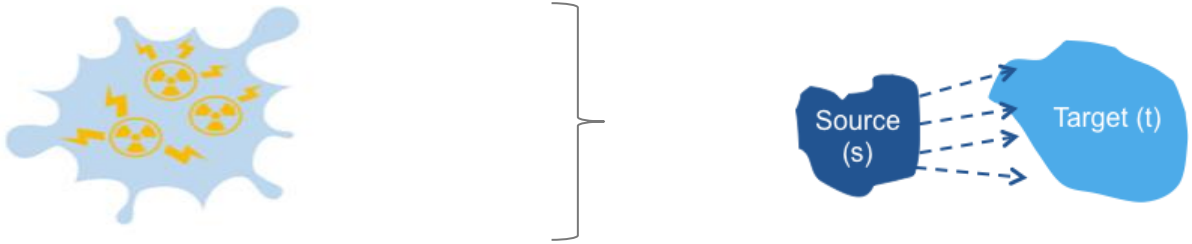
PLAN A

- Scientific view
- Technical view
- Foreseen solution
- Infrastructures
- Tools
- First results
- Conclusion

PLAN B

- Start the talk
- See how it goes
- ☺

Some context: what do we want to do?

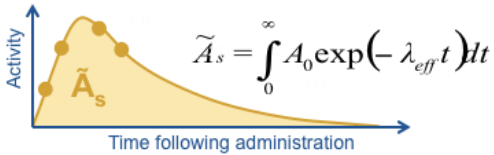


Tumoral cell

Organs

$$D_{t \leftarrow s} = \tilde{A}_s \times S_{t \leftarrow s}$$

Cumulated activity



$$\tilde{A}_s = \int_0^{\infty} A_0 \exp\left(-\lambda_{eff} t\right) dt$$

- Bio-kinetics and uptake distribution
- Patient-specific

S-value (dose factor)

$$S(r_t \leftarrow r_s) = \sum_i \frac{\Delta_i \Phi_i(r_t \leftarrow r_s)}{m_t}$$

- Nuclear decay data
- Source/target geometry

The OpenDose collaboration

Challenges

- 2 ICRP 110 reference adult phantoms (male and female) and more to come (pediatric and next generation mesh-based phantoms)
- 140 organs (19600 target/source combinations!)
- ICRP 107: ~1200 radionuclides
- MIRD RADTABS source of decay data: ~300 radionuclides

Too big for a single institution!!!

Proposal

- Collaborative work, everyone is welcome!
- Generate data with different Monte Carlo codes to cross-verify data
- Generate Specific Absorbed Fractions with associated uncertainties
- Traceable and reproducible data
- Create a free database
- Create an easily accessible website
- Compute S-values with uncertainties from SAFs

And what's the matter?

- **1 simulation = 1 Gate/Geant4 job**
  - `Gate -a [Source_ID,95][particle,gamma][energy,1][nb,10e5] main_AF.mac`
- **50 960 simulations**
  - 140 source organs, 2 particle types, 91 energy levels, 2 models
- **On a local cluster (240CPU) :**
  - 1 organ x 2 particles x 91 energies x 1 model = 1 day

More than 1 million CPU hours

Where we start from, where we go

- A computational model
  - Parametric, independent simulations
  - 50,960 simulations = 50,960 jobs
  - « Embarrassingly Parallel » problem

- A local cluster
  - 240 CPU
  - 280 days of computing

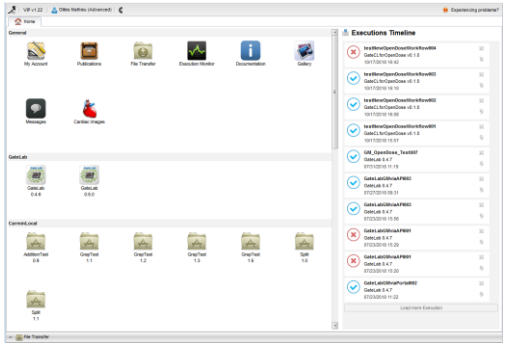
- Grid infrastructure
  - Adapted model
  - Resources ++
  - Available tools

Solution

- Infrastructure

Together, we'll be many!

- Tools



Gate/Geant4 on the grid

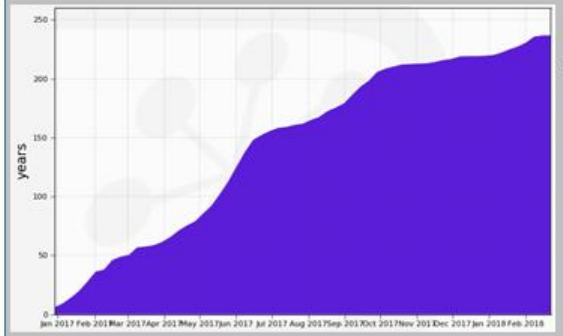
Web portal

Application as a service
File transfer to/from grid

VIRTUAL IMAGING PLATFORM

Infrastructure

Supported by EGI Infrastructure
Uses biomed VO (~65 sites in Europe and beyond)
230 cumulated CPU years utilized by VIP applications in 1 year

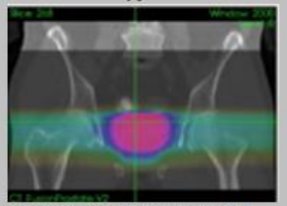


France-Grilles

DIRAC

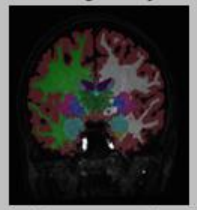
Scientific applications

Cancer therapy simulation



Prostate radiotherapy plan simulated with GATE(L. Grevillot and D. Sarrut)

Neuro-image analysis

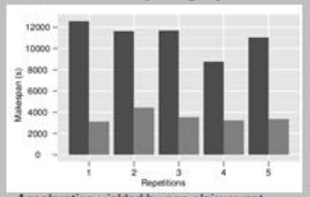


Brain tissue segmentation with Freesurfer

Image simulation

Echocardiography simulated with FIELD-II (O. Bernard *et al*)

Modeling and optimization of distributed computing systems



Acceleration yielded by non-clairvoyant task replication (R. Ferreira da Silva *et al*)

Users

1000+ registered users in January 2018
44 publications since 2011

GateLab

GateLab allows you to submit your GATE simulations on EGI from a simple web page:

- Upload your data and main macro file from the web browser.
- Select the estimated CPU time needed to complete your simulation.
- Choose the GATE release.
- After completion, results are automatically merged and ready for download.

OpenDose requires the new DoseByRegions output:

→ Need to update the GATE release to the latest version 8.1

→ Need to update the merger

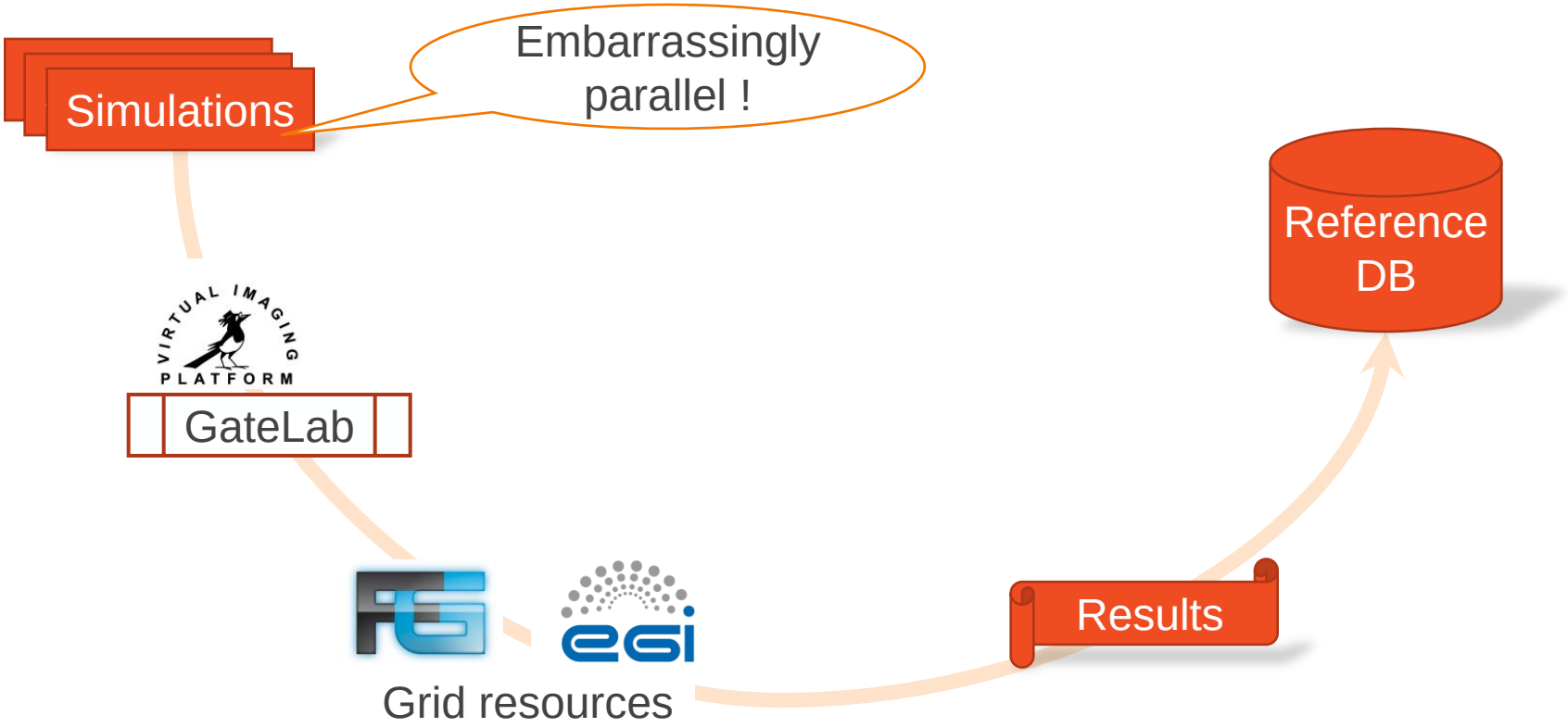
GateLab

- Update of the GATE release
  - DockerFile which build a new image with Geant4, ROOT and GATE on CentOS.
  - Script to extract the GATE binary and dependencies from the Docker image.
  - Add a env.sh to ease the setup of Geant4 and ROOT environment variables.

GATE release 8.1 is now available

- Update of the merger for the DoseByRegions output
  - Almost finished.

To summarise…



Nice. However…

- **Generate 50 960 configuration files?**

Thou shalt use parameters

→ A NEW WORKFLOW

- **Manually launch 50,960 jobs through the portal?**

Thou shalt script

→ A CLIENT CODE

Workflow description through Boutiques

Describe | Publish | Integrate | Execute

Inter-platform, command line applications.

- Polyvalent JSON format
- Linux containers

- https://github.com/boutiques

An OpenDose application using Boutiques

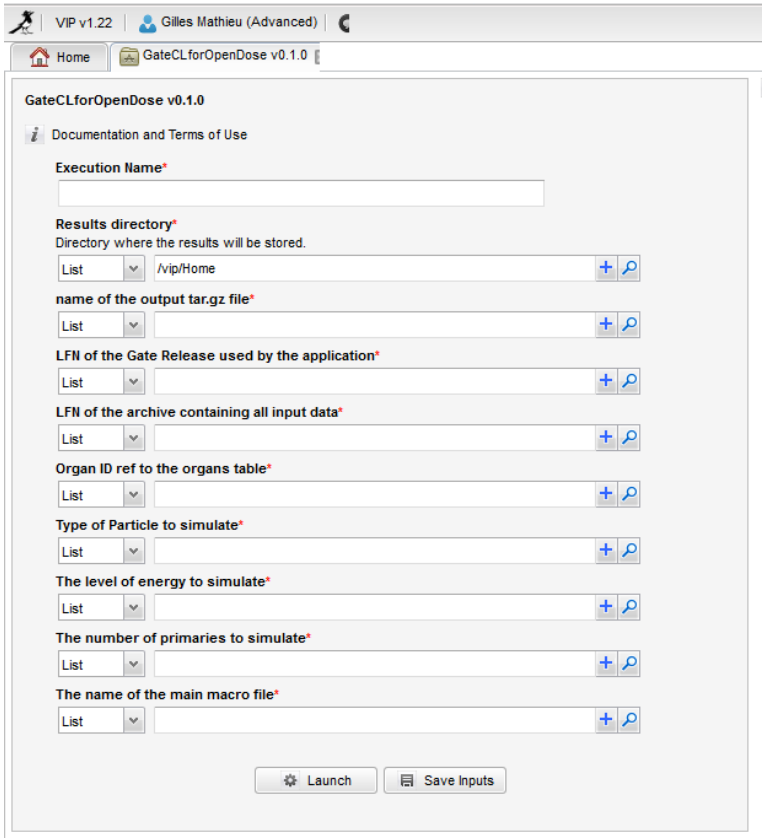
- A JSON file describing:
  - The command line itself

```
"command-line": "tar -zxf [GATERELEASE]; unzip [INDATA];

tar -zxvf gate_shared_libs.tar.gz; source ./init_env.sh;

./Gate -a [Source_ID,[ORGANID]] [particle,[PARTICLETYPE]] [energy,[ENERGY]] [nb,[NBPRIMARIES]]
[MACFILE] > output.log;

tar czf [RESULTS] ./output output.log",
```

  - Used parameters

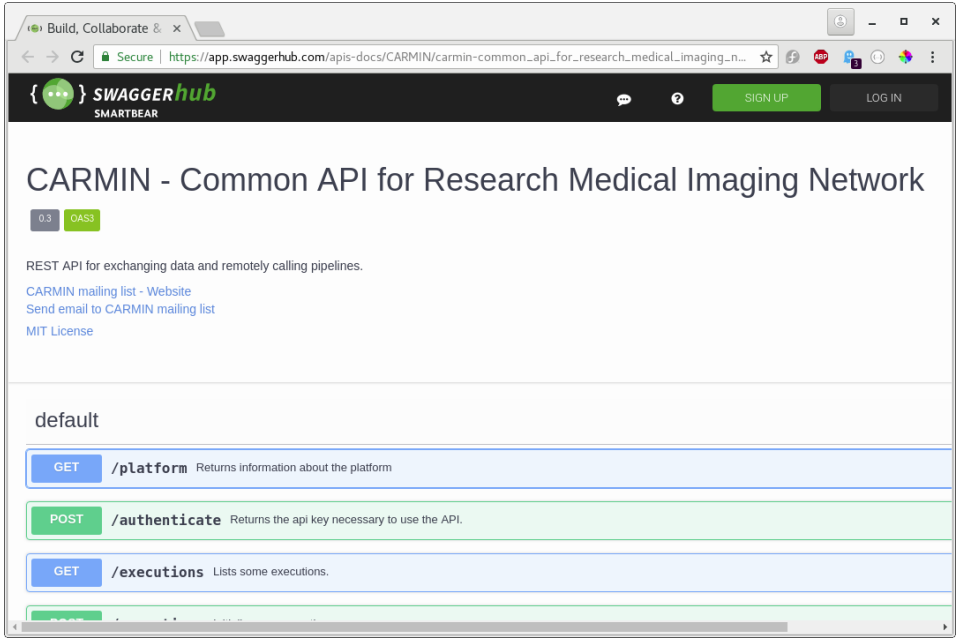
```
"inputs": [
{ "id": "gaterelease",
 "name": "LFN of the Gate Release used by the application",
 "optional": false,
 "type": "File",
 "value-key": "[GATERELEASE]"}, (…)]
```

An OpenDose application using Boutiques



The CARMIN API

- https://github.com/CARMIN-org
- https://app.swaggerhub.com/apis/CARMIN



An OpenDose client using CARMIN

```
public class OpenDoseClientClass {
  public static void main(String[] args) throws ApiException {
    /********** INIT API CLIENT ***********/
    ApiClient vipApiClient = new ApiClient();
    vipApiClient.setApiKey("thisisadummykey");
    vipApiClient.setBasePath("http://vip.creatis.insa-lyon.fr/rest");
    DefaultApi vipApi = new DefaultApi(vipApiClient);
    /********** SET PIPELINE AND LAUNCH EXECUTION ***********/
    Execution execution = new Execution();
    execution.setPipelineIdentifier("GateCLforOpenDose/0.1.0");
    Map<String, Object> inputValues = new HashMap<>();
    inputValues.put("indata", gateInputLFN);
    inputValues.put("gaterelease", gateReleaseLFN);
    inputValues.put("nbprimaries", numberOfPrimaries);
    inputValues.put("macfile", macFileName);

    // loop over all organs found in input matrix
    for (String organ : organsList) {
        inputValues.put("organid", organ);
        // loop over all particle types
        for (String particle : particlesList) {
               inputValues.put("particletype", particle);
               // loop over all energy levels
                   for (String energy : energiesList) {
                       inputValues.put("energy", energy);
                       executionName = "OpenDose_" + organ + "_" + particle + "_" + energy;
                       inputValues.put("outfilename", executionName + ".tar.gz");
                       // setup and launch execution
                       execution.setInputValues(inputValues);
                       execution.setName(executionName);
                       execution = vipApi.initExecution(execution);
                   }
        }
    }
  }
}
```

Initialisation

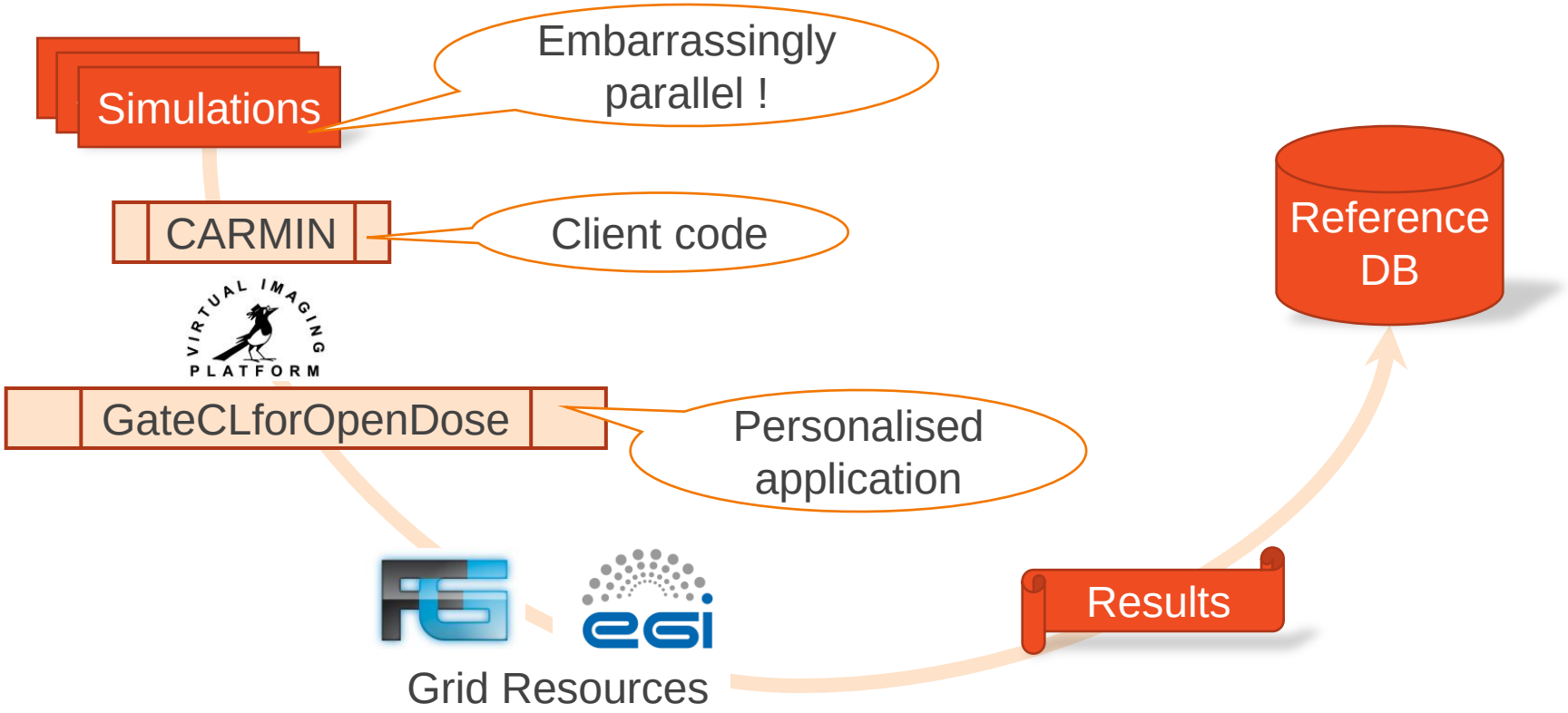
Application definition

Passing parameters

loops

1 organ
+ 1 particle
+ 1 energy level
= 1 submitted job

To summarise… (v2.0)



Where are we now?

- Global workflow analysis

- Submission tests through GateLab

- Draft client code

- Dedicated application deployed and working on VIP

- Production scale tests

- Needed adaptations!

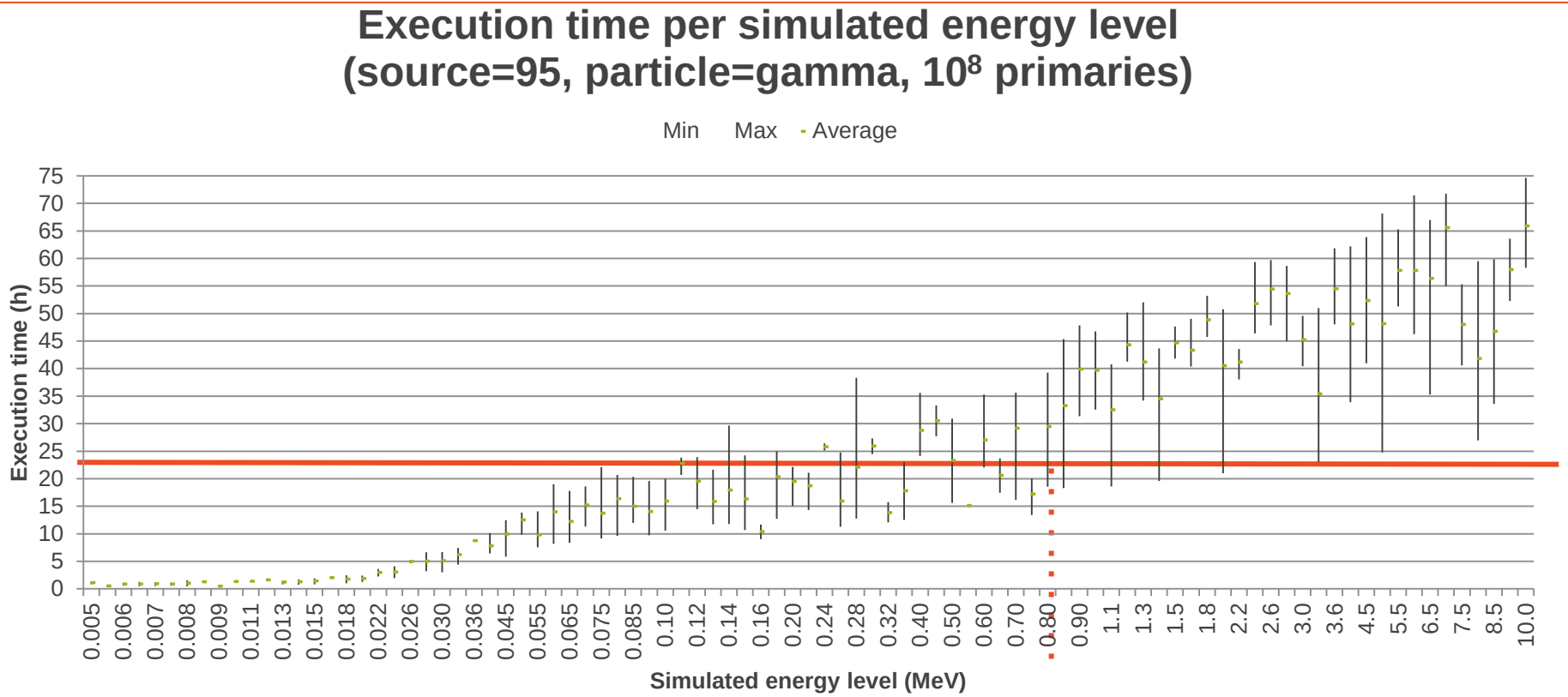
- Production

- Results gathering

Needed adaptations ?

- Long jobs (>24h) don’t run well on the grid
- GOOD NEWS: GateLab has a mechanism to split jobs
- BAD NEWS: GateCLforOpenDose doesn’t

A quick look on execution times



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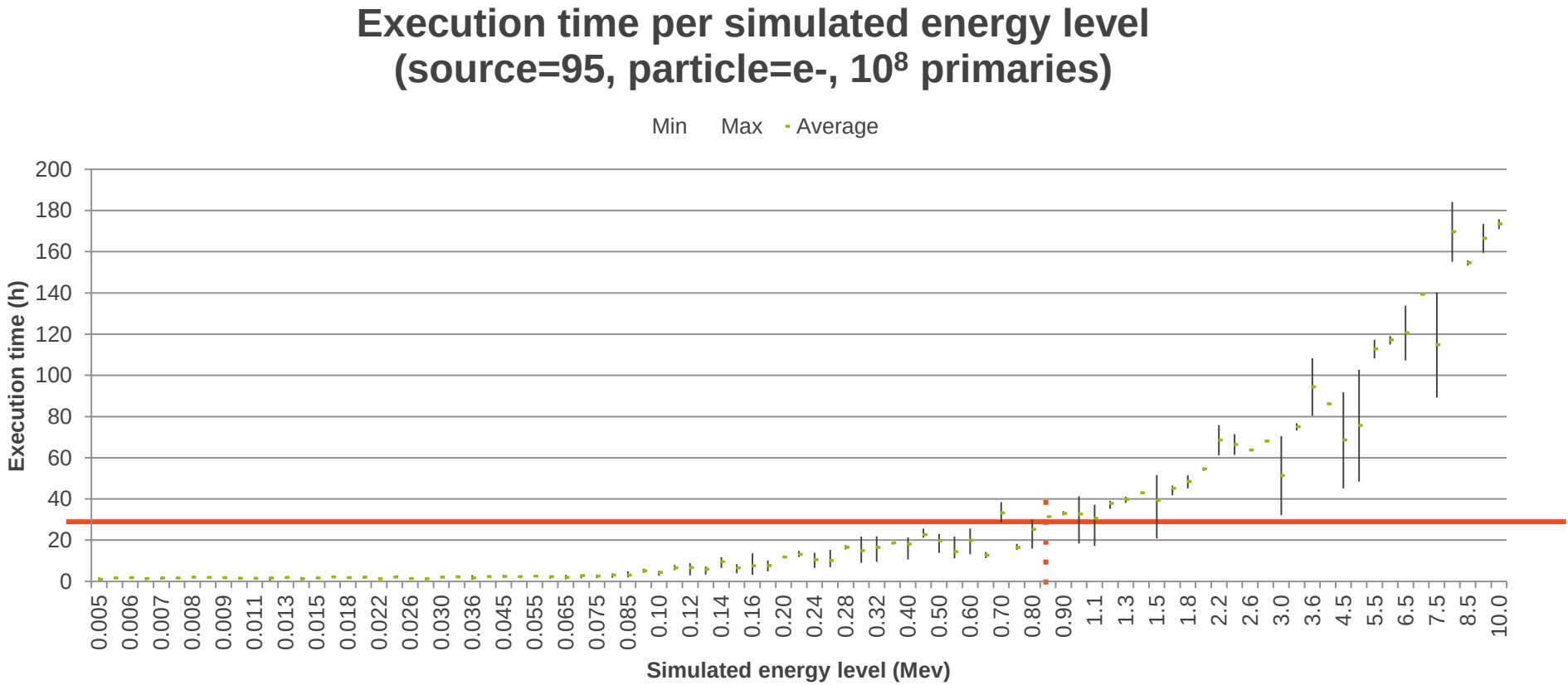


Houston, we have a problem

- Only 2/3 of the overseen production can run smoothly in current situation
  - Simulations with energy level < 0.8Mev
- We need to either:
  - Implement a split mechanism in our application
  - Modify GateLab
- WORK IN PROGRESS! Keep tuned ;-)

Meanwhile…

- We have started with REAL production anyway
  - All source organs, e- and gamma
  - Male and Female model

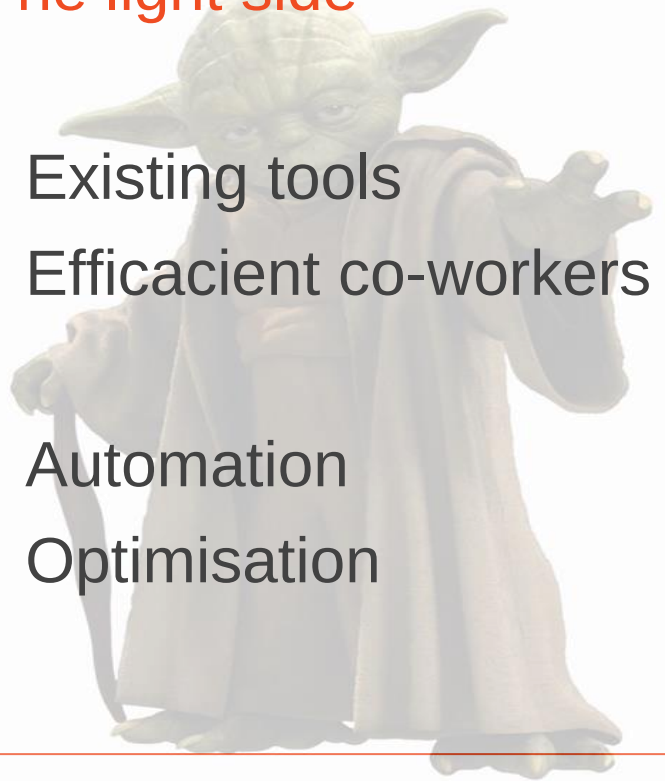
- Submission started Tuesday afternoon (11.Dec.)
  - Around 2000 simulations finished, and counting

A first feedback

The light side

- Existing tools
- Efficacient co-workers

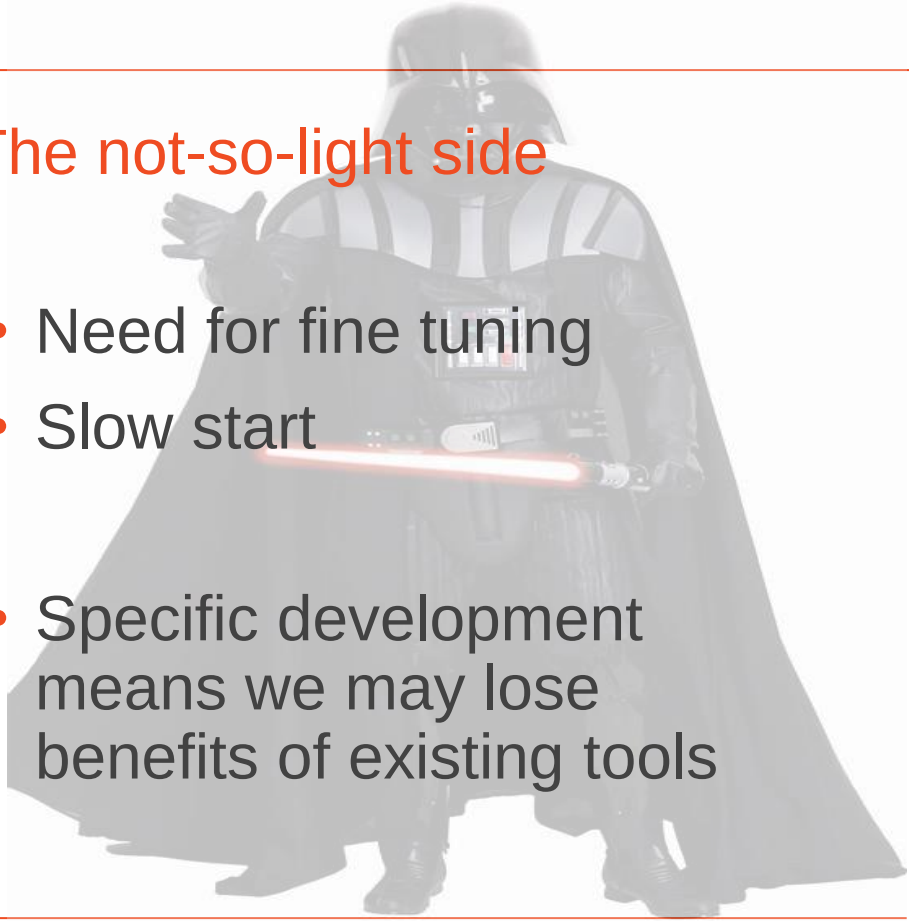
- Automation
- Optimisation



The not-so-light side

- Need for fine tuning
- Slow start

- Specific development means we may lose benefits of existing tools



To the future, and beyond

- **Industrialisation**
  - Optimise code and submission
  - Use more/different models
  - Ensure reproducibility et traceability

- **Scientific exploration**
  - Re-use submission framework
  - Test other MC softwares

- **Technical Exploration**
  - Other tools?
  - Other infrastructures?

Computing@OpenDose in a nutshell

Radioisotope

Tumoral cell

Models

Holy Grail!

Reference DB

Simulations

Nice tools

Grid

Results

Inserm

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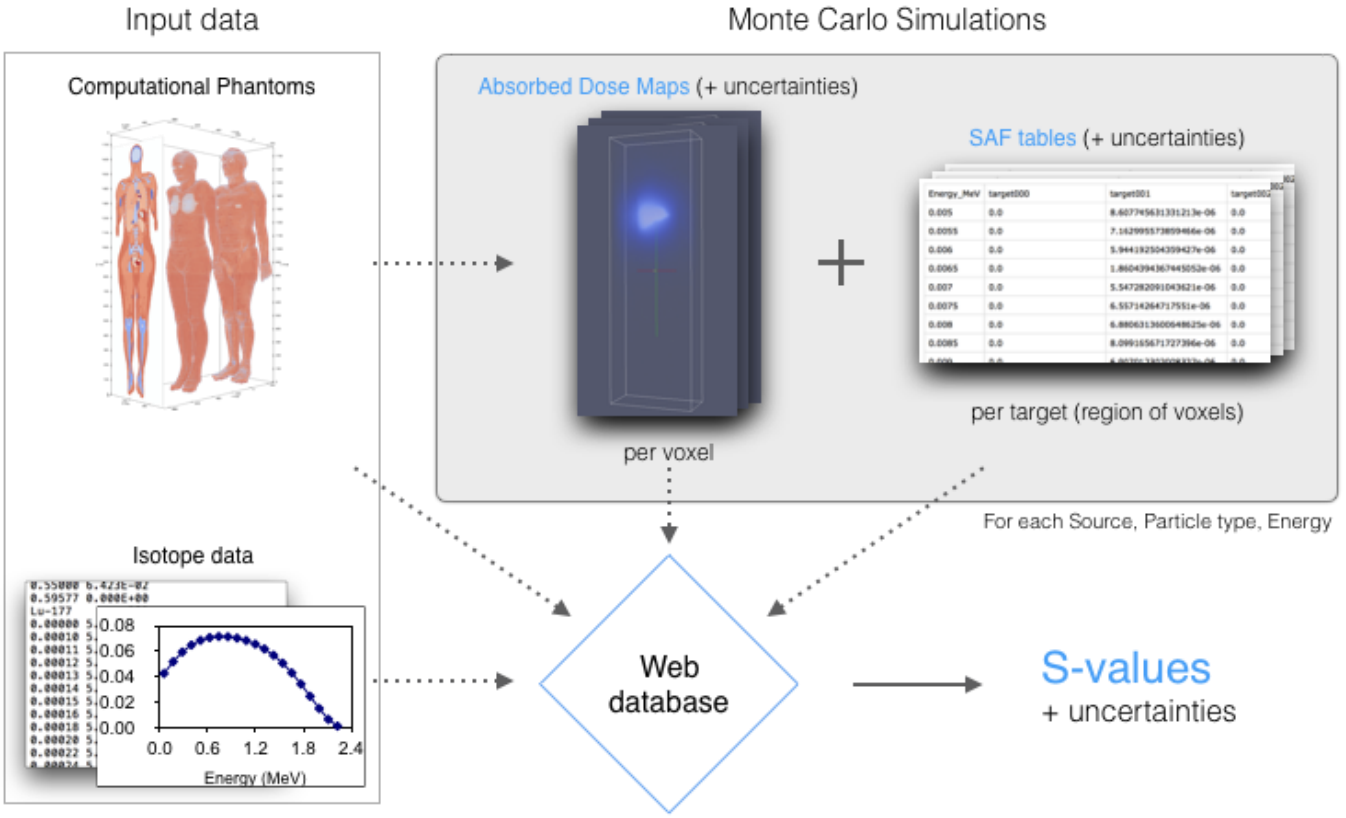
From science to health

Annexes

Informations, links & references for an offline reading

The OpenDose collaboration



More on OpenDose

- MCMA2017 talk by M.Chauvin
  - http://people.na.infn.it/~mettivie/MCMA%20presentation/18%20Aula%20Magna/9_45_Chauvin.pdf

- MRTDosimetry2018 talk by M.Chauvin
  - http://mrtdosimetry-empir.eu/wp-content/uploads/2018/10/13_MRTdosimetryWorkshop_Chauvin.pdf

France Grilles

- Une offre de services sur une infrastructure informatique distribuée pour le calcul et le stockage de données scientifiques
- Une équipe d'animation au service de l'ensemble des acteurs qui coordonne les opérations de cette infrastructure basée sur les technologies de grille et de cloud informatiques
- Une communauté de plus d'un millier d'utilisateurs dynamiques, prêts à partager leurs connaissances et à s'entraider
- Le représentant de la France au niveau international au sein d'EGI
- Et surtout et avant tout un réseau résolument humain !
- www.france-grilles.fr

EGI

- www.egi.eu

Boutiques

- Décrire, publier, intégrer et exécuter des applications en ligne de commande inter-plateformes.
  - faciliter le portage d'applications
  - import et échange d'applications
  - science ouverte et reproductible

- Format JSON polyvalent pour décrire la ligne de commande, les entrées et les sorties
- Utilisation de conteneurs Linux pour faciliter l'installation et le partage d'applications
- https://github.com/boutiques

Portage des jobs OpenDose sur la grille

- Code client pour utiliser VIP via CARMIN
  - https://github.com/CISI-INSERM/OpenDose-Computing/tree/master/VIPclient

- Descripteur JSON pour portage de la ligne de commande OpenDose dans VIP via Boutiques
  - https://github.com/CISI-INSERM/OpenDose-Computing/tree/master/Boutiques

Crédits

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