



# The role of Computational Geosciences in the Data Science paradigm

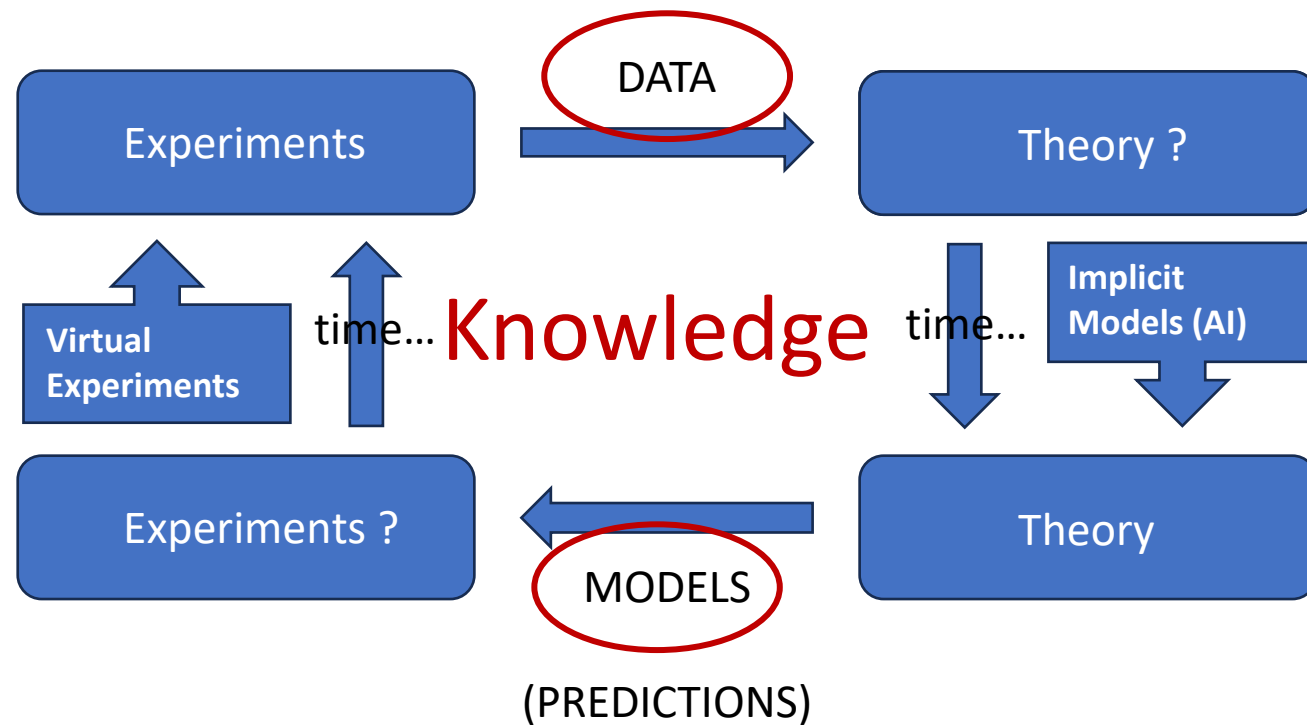
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Istituto Nazionale di Geofisica e Vulcanologia

OpenData Workshop, November 15, 2023

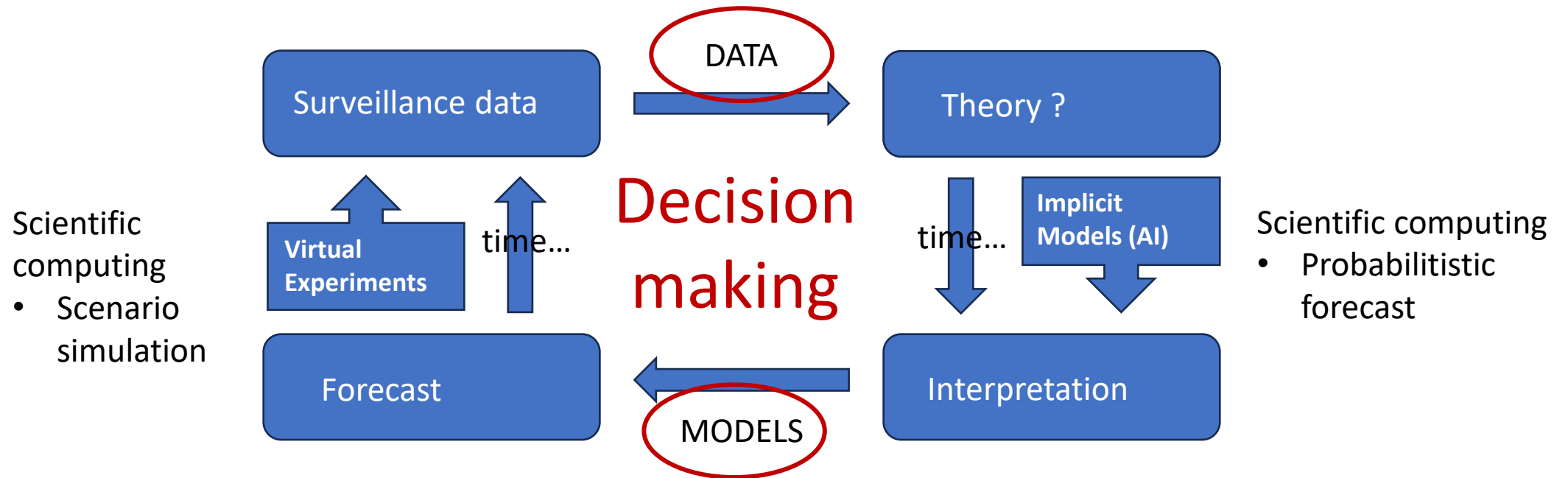


- Scientific computing
- more statistics!
  - *extremes*



- Scientific computing
- reduce data

**Acceleration of scientific knowledge !!**  
**⇒ Digital Twins**

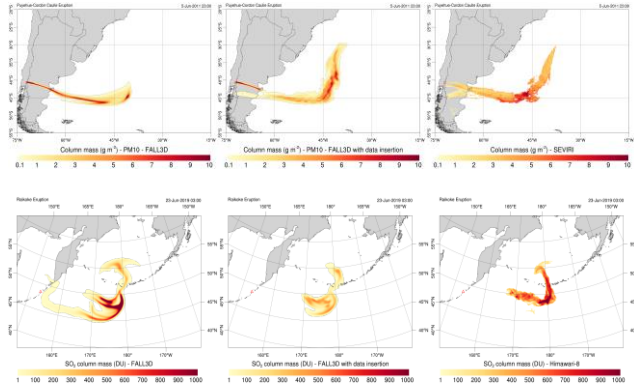


## Urgent Computing!!

(sensitive information: Data/Model policy issues)



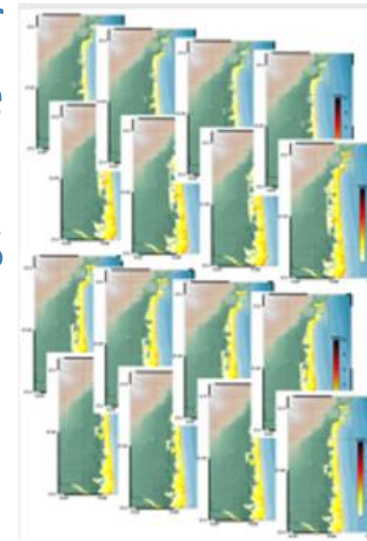
# In silico experiments



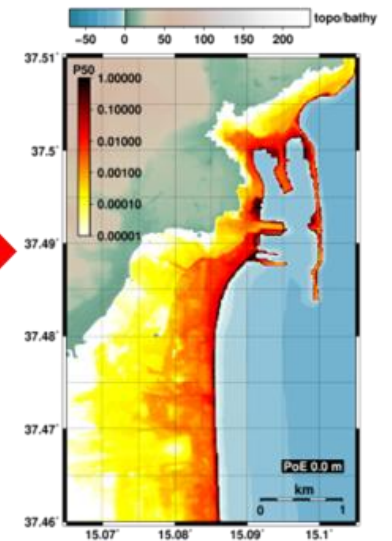
More data  
(assimilation)

Larger  
Ensemble size  
Simulation of  
EXTREMES

Inundation scenarios

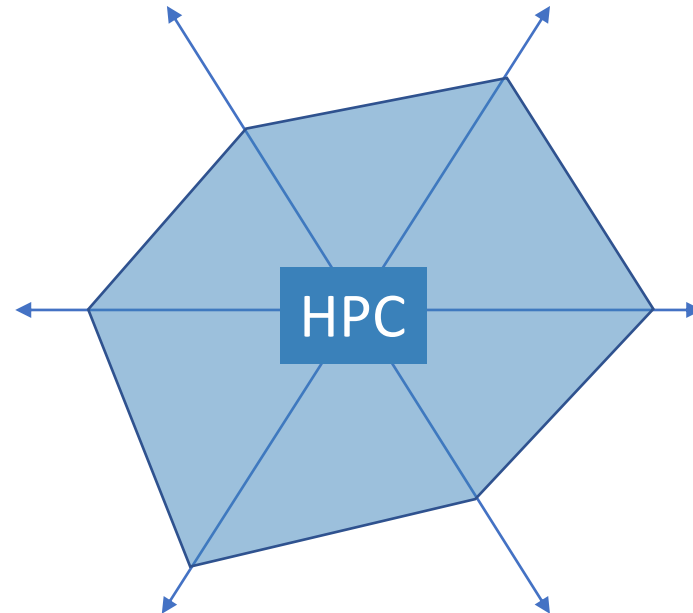


Local hazard map



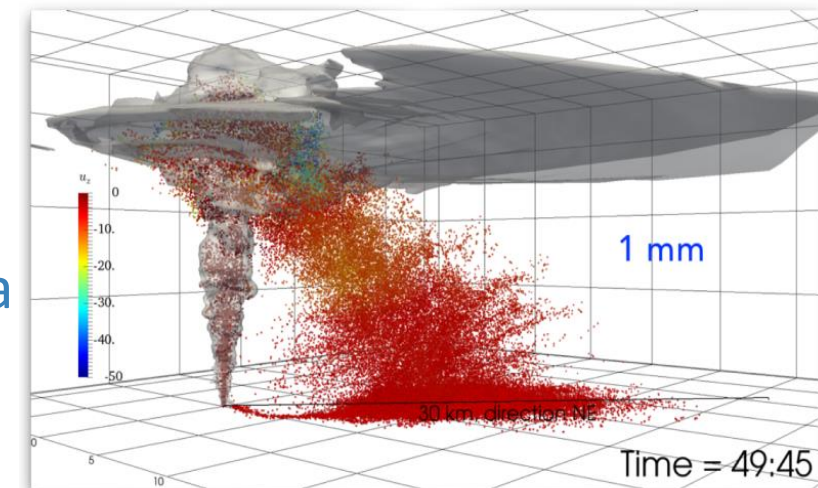
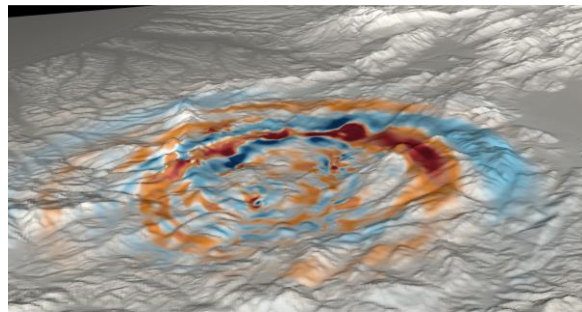
Larger spatial/temporal  
domains

Higher spatial/temporal resolution

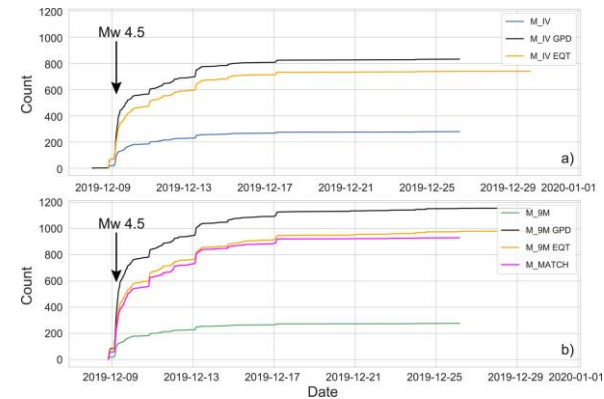
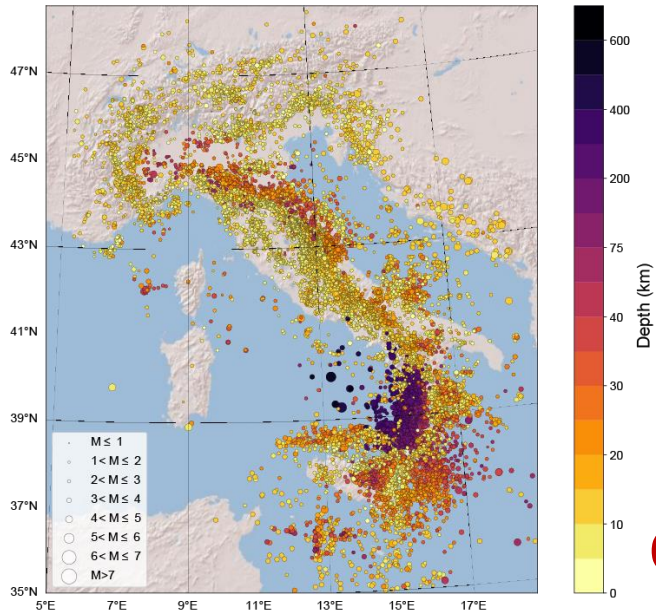


More physics  
(increase complexity)

More output data  
(analysis)

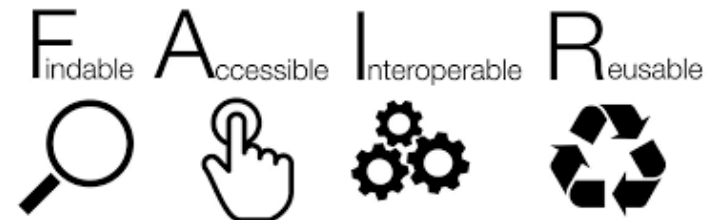


compromise between *storing (simulation data lakes)* and *producing on demand* simulation data yet to be found



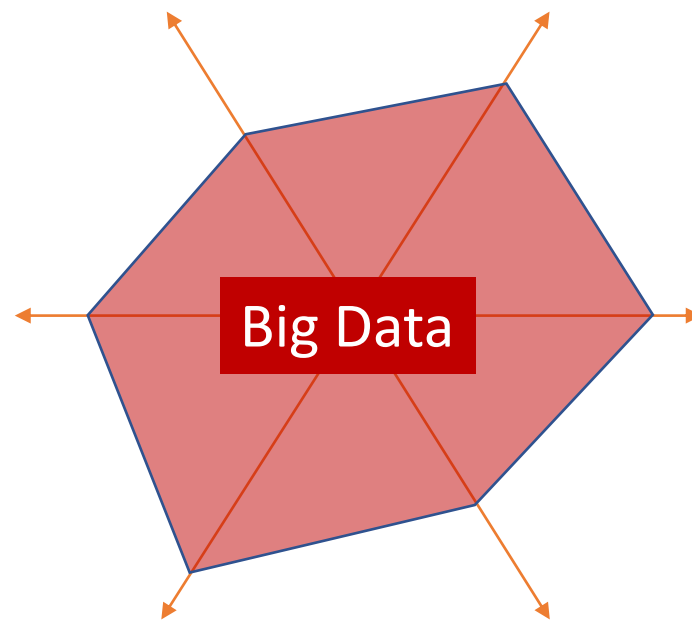
Increased Data volumes

Increased Data sources (Internet of Things)



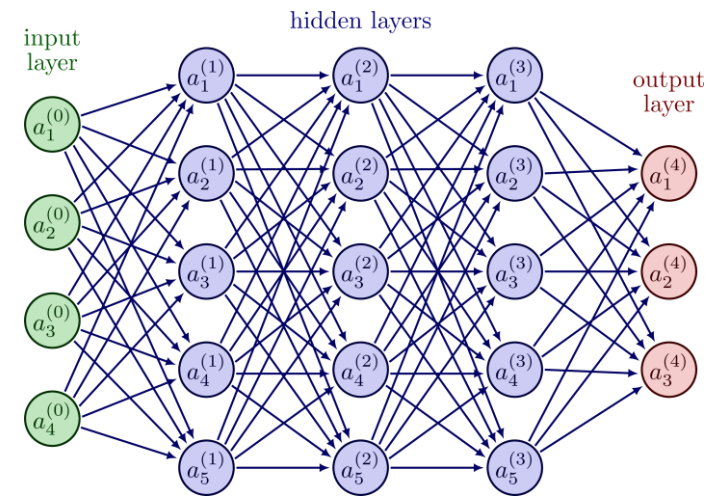
Quality standards

Enhanced interoperability



Improved Network capabilities

Evolved ML / AI techniques





# Conclusion

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- ❑ **Data Science** paradigm will accelerate scientific discovery
- ❑ **Scientific Computing** is serving to:
  - Transform the data (for the theory)
  - Reduce the data (implicit modeling)
  - Produce new data (especially for *extremes*)
- ❑ The **quality of the data** (and, thus, of the **software**) is a key issue.
- ❑ Software (as a *Digital Asset*) should also be FAIR!
  
- ❑ **Urgent Computing** will be a critical testbed for such issues.

# Il Centro per le Geoscienze Computazionali



# Pillar 1) Favorire l'accesso alle risorse di calcolo e di analisi dati, e loro armonizzazione

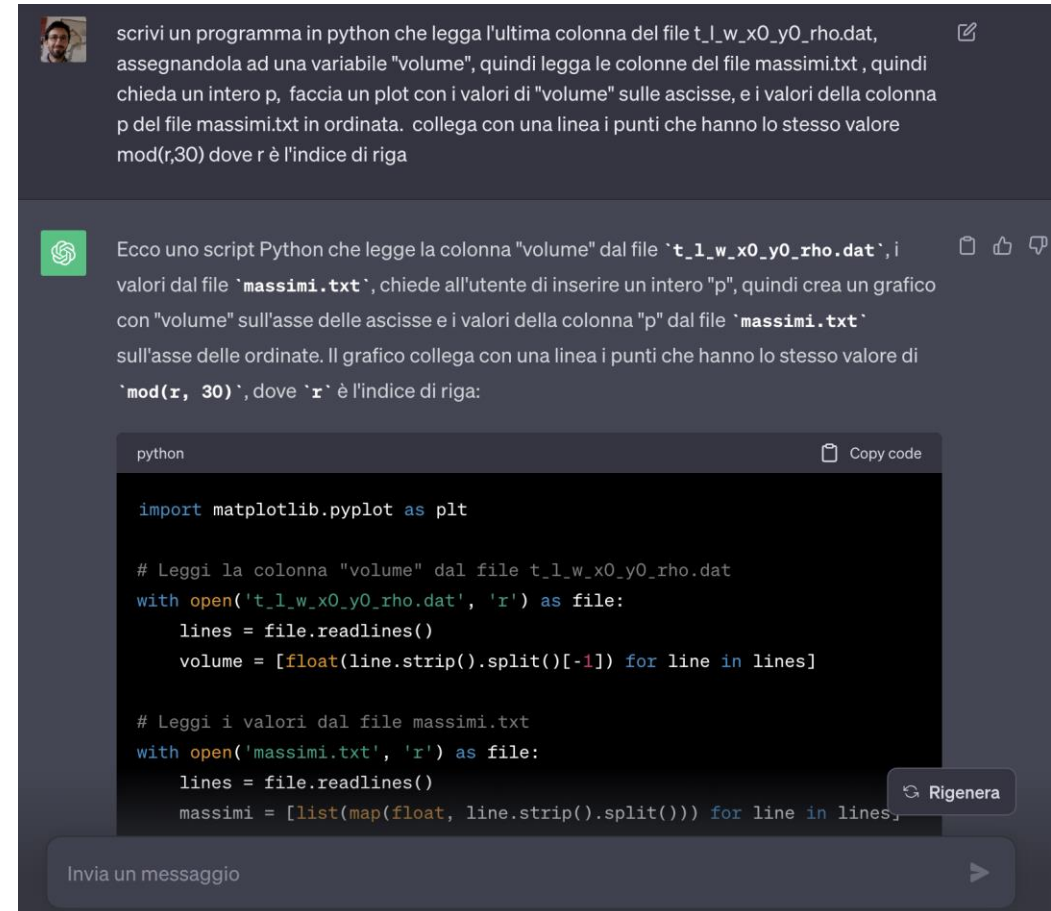
- Mantenere e gestire un sistema di calcolo di livello Tier3, per dare accesso a risorse (*hardware*) di calcolo ed analisi dati ad alte prestazioni alla comunità scientifica e tecnologica dell'Ente.
- Dare accesso a risorse *software* HPC/HPDA/AI.
- Promuovere l'ottimizzazione e l'armonizzazione delle risorse distribuite presso le Sezioni INGV, di concerto con il CSI (Centro Servizi Informatici), con i gruppi di lavoro di Istituto e le Unità Funzionali associate ai Centri di Elaborazione Dati (CED) di Sezione.
- Coordinare lo sviluppo delle risorse HPC/HPDA/AI dell'INGV in una prospettiva di scalabilità e sostenibilità economica ed ambientale.





# Pillar 2) Potenziamento delle competenze (capacity building)

1. Coordinare le iniziative di formazione del personale, e condividere le conoscenze nell'ambito HPC/HPDA/AI.
2. Far crescere la comunità HPC/HPDA/AI dell'INGV, facilitando lo sviluppo tecnologico, il *porting* ed *enabling* di applicazioni ad alte prestazioni.
3. Supportare i servizi HPC/HPDA/AI dell'INGV per la valutazione della pericolosità associata a fenomeni geofisici, vulcanici ed ambientali.



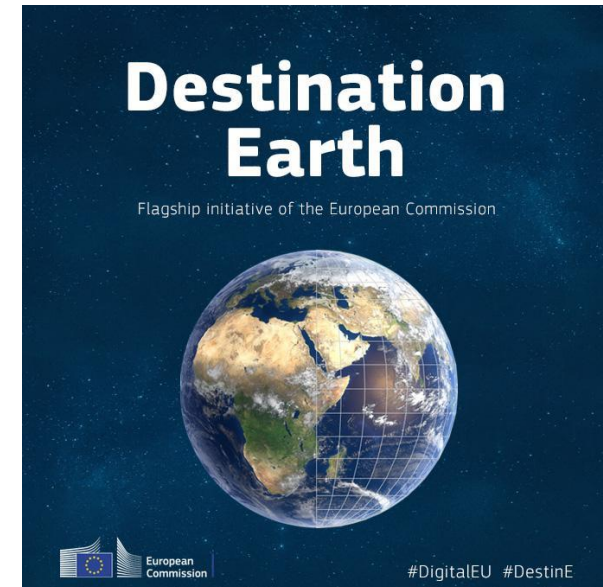
The screenshot shows a chat conversation. The user asks for a Python program to read the last column of a file, assign it to a variable 'volume', read the columns of another file 'massimi.txt', ask for an integer 'p', create a plot of 'volume' vs 'p', and connect points with lines every 30 rows. The AI response provides a Python script that does exactly that. The script uses 'matplotlib.pyplot' for plotting and 'open()' to read the files. It also includes a 'Rigenera' button and a 'Copy code' button.

```
python  
import matplotlib.pyplot as plt  
  
# Leggi la colonna "volume" dal file t_1_w_x0_y0_rho.dat  
with open('t_1_w_x0_y0_rho.dat', 'r') as file:  
    lines = file.readlines()  
    volume = [float(line.strip().split()[-1]) for line in lines]  
  
# Leggi i valori dal file massimi.txt  
with open('massimi.txt', 'r') as file:  
    lines = file.readlines()  
    massimi = [list(map(float, line.strip().split())) for line in lines]
```

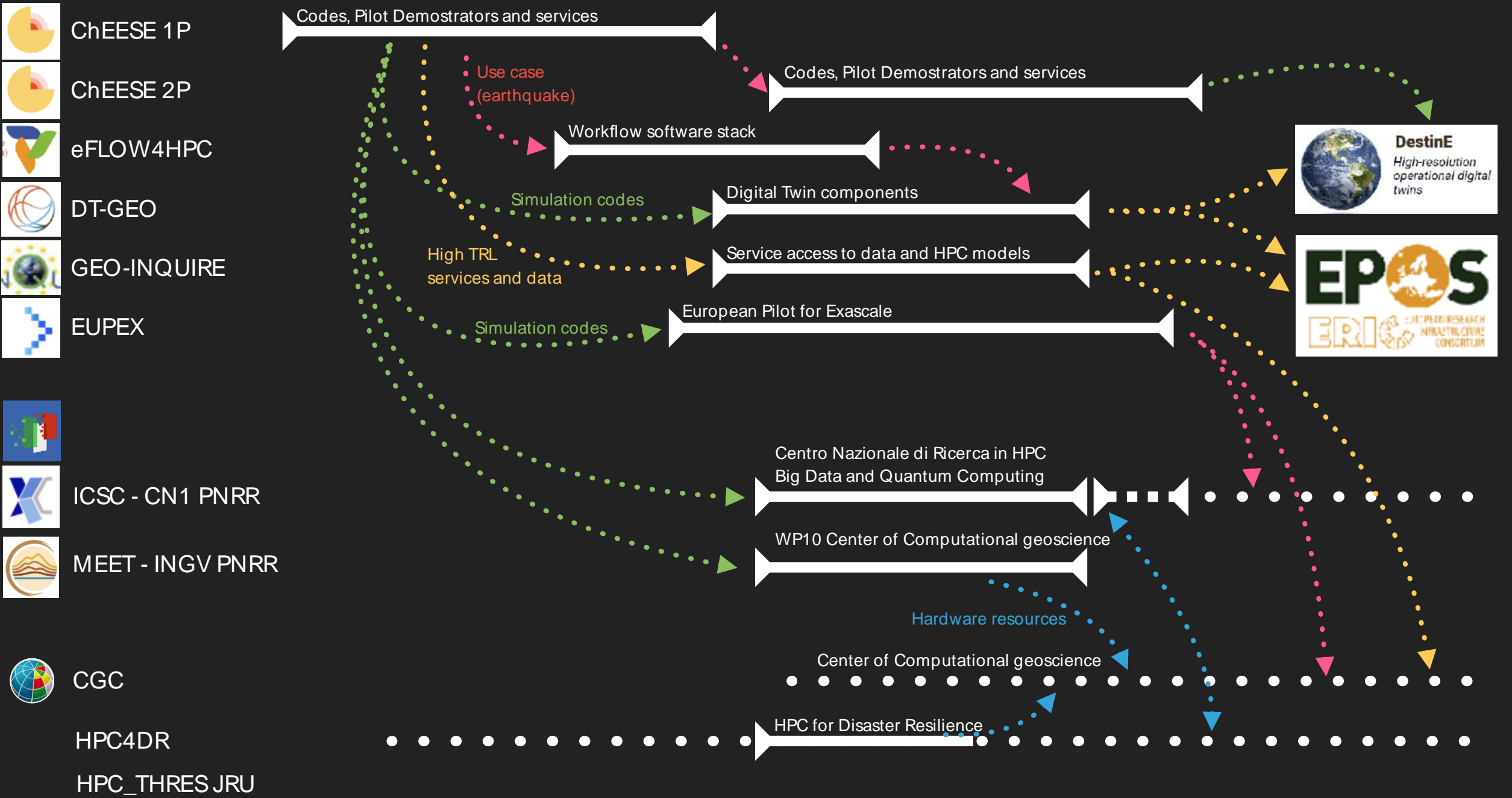
(Intelligenza Artificiale: oltre ChatGPT!)

# Pillar 3) Integrazione con l'ecosistema HPC Nazionale ed Europeo

1. Fornire servizi di Accesso Virtuale e Transnazionale (Virtual and Transnational Access) alle risorse HPC/HPDA/AI per gli ERIC (in particolare EPOS e EMSO), per i progetti con partecipazione INGV che lo prevedono, e per la comunità scientifica di riferimento.
2. Facilitare l'accesso alle risorse HPC/HPDA/AI di livello superiore in ambito Regionale, Nazionale ed Europeo.
3. Integrare la strategia INGV con le iniziative della EOSC (European OpenScience Cloud) a livello Nazionale ed Europeo.
4. Supportare le attività a scala Europea (Horizon Europe) ed in particolare le attività progettuali legate ad EuroHPC e a Destination Earth.



2018 2019 2020 2021 2022 2023 2024 2025 2026 2027 2028 2029

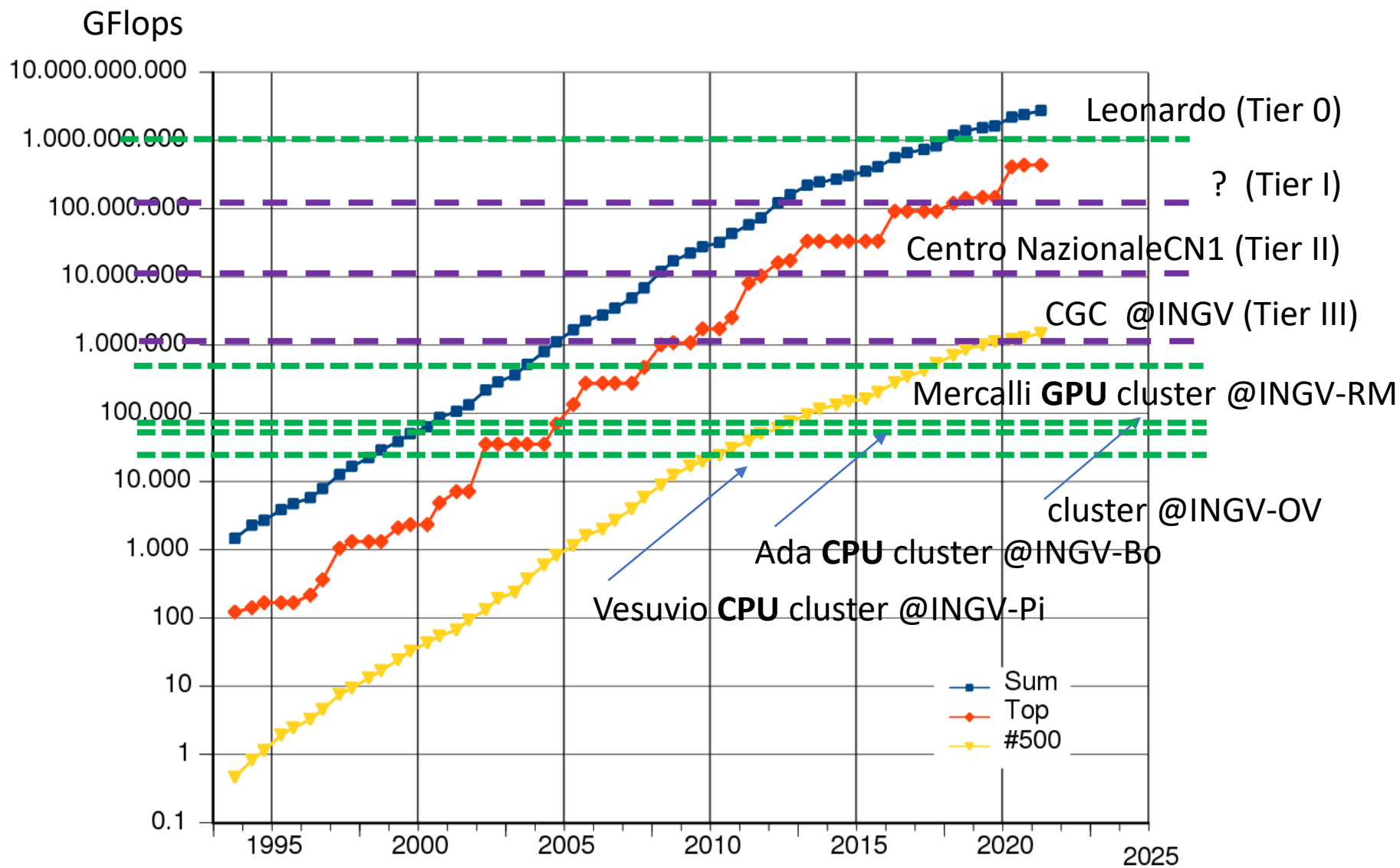




# HPC@INGV vs TOP500 2021 supercomputers

1 FLOPs  
= 1 Floating-point operation / s

G = Giga ( $10^9$ )  
T = Tera ( $10^{12}$ )  
P = Peta ( $10^{15}$ )  
E = Exa ( $10^{18}$ )



# HPC@INGV ecosystem and strategy

Target	Risorse di calcolo	Target	Sostenibilità
~ <b>exaFLOPS</b>	<ul style="list-style-type: none"> <li>Centres of Excellence</li> <li>PRACE</li> </ul>	<ul style="list-style-type: none"> <li>Scientific excellence (grand challenges)</li> <li>Urgent computing</li> <li>Probabilistic hazard assessment / forecast /early warning</li> </ul>	European Commission (Long-term?)
~ <b>10 petaFLOPS</b>	<ul style="list-style-type: none"> <li>Centro Nazionale HPC</li> </ul>	<ul style="list-style-type: none"> <li>Hazard and risk assessment for natural catastrophes (<b>High TRL</b>)</li> <li>Service to the society (<b>High TRL</b>)</li> </ul>	<ul style="list-style-type: none"> <li>PNRR</li> <li>?</li> </ul>
~ <b>1 petaFLOPS</b>	<ul style="list-style-type: none"> <li>Centro Geofisica Computazionale INGV</li> </ul>	<ul style="list-style-type: none"> <li>Fundamental research (<b>Low TRL</b>)</li> <li>Service to the scientific community (<b>Intermediate TRL</b>)</li> </ul>	<ul style="list-style-type: none"> <li>PNRR</li> <li>Progetti Infrastrutturali</li> <li>Servizi HPC</li> </ul>
~ <b>10-100 teraFLOPS</b>	<ul style="list-style-type: none"> <li>Sezioni INGV (<b>federazione</b>)</li> </ul>	<ul style="list-style-type: none"> <li>Fundamental research and development (Low TRL)</li> </ul>	<ul style="list-style-type: none"> <li>Progetti PON</li> <li>EOSC</li> <li>Fondi ordinari</li> </ul>

