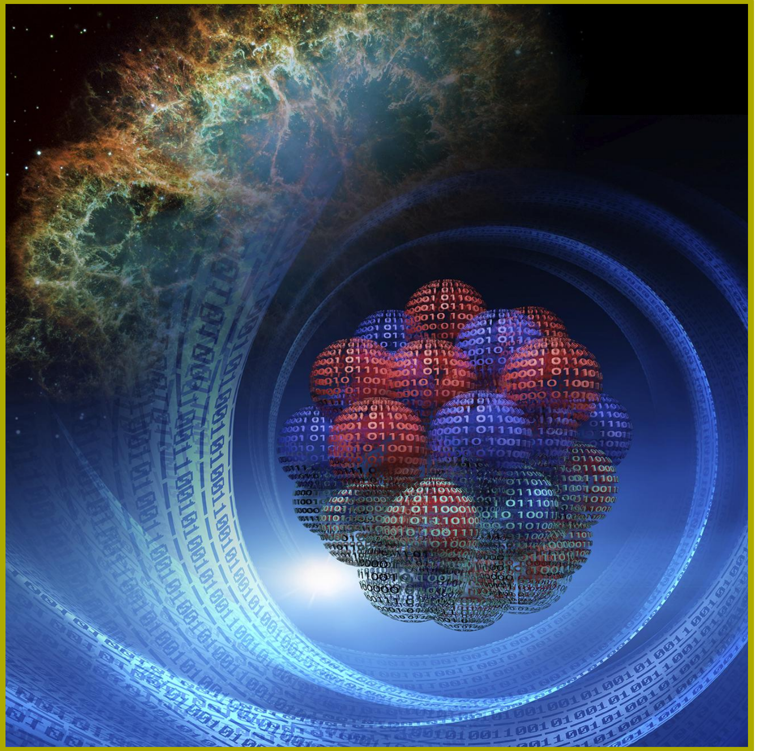
WOUTER RYSSENS


Andy Sproles, ORNL

# Nuclear Astrophysics

## from the microscopic description of nuclei to the macroscopic explosion of stars

W. Ryssens and S. Goriely

April 21st 2023

wryssens.com

wryssens@ulb.be

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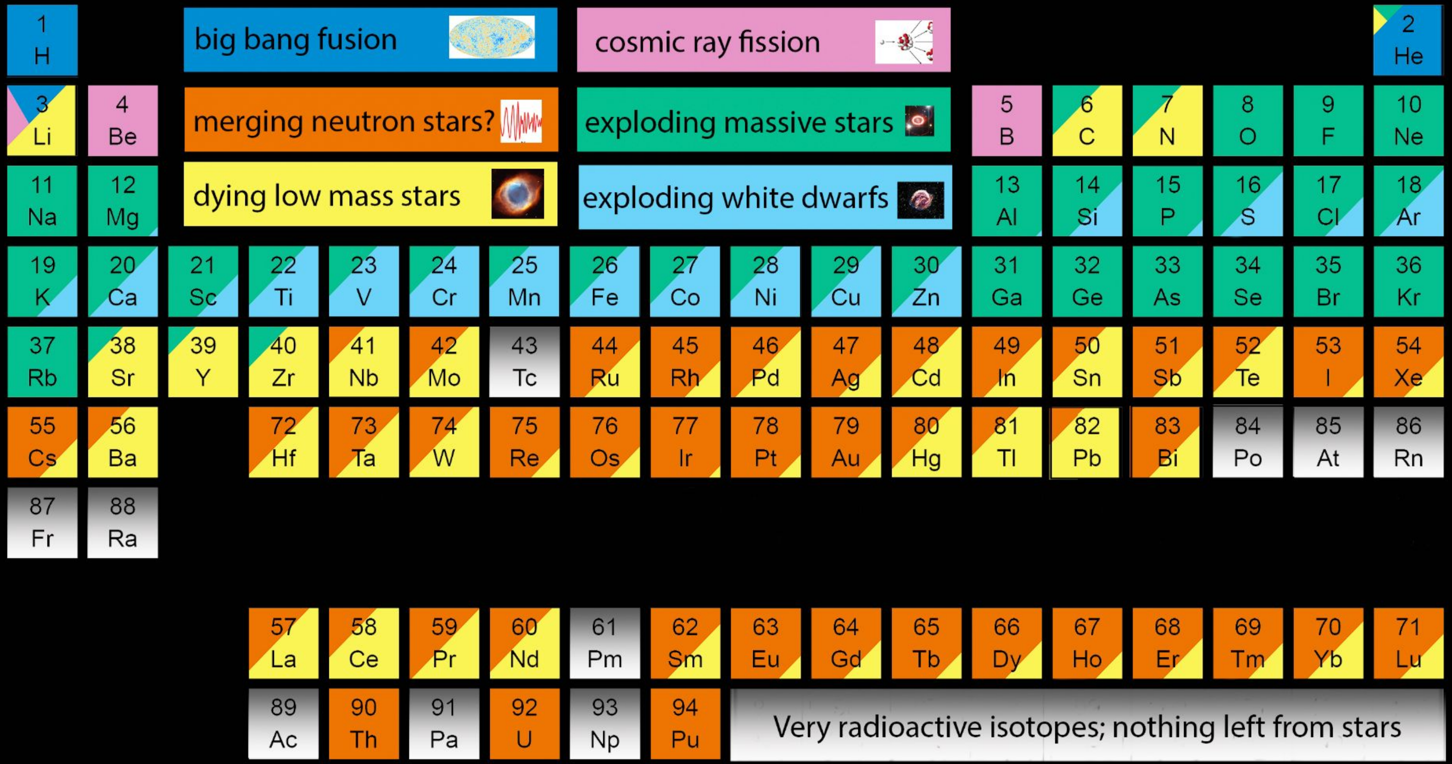
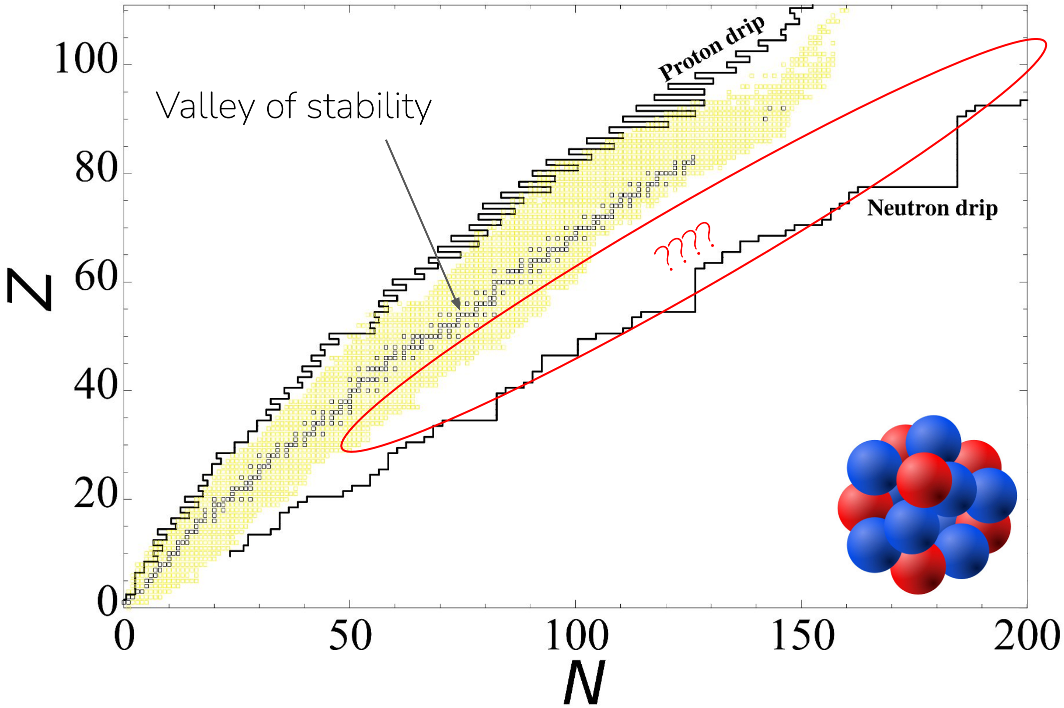



Graphic created by Jennifer Johnson
http://www.astronomy.ohio-state.edu/~jaj/nucleo/

Astronomical Image Credits:
ESA/NASA/AASNova

# The nuclear chart...

Different **elements**




Different **isotopes**

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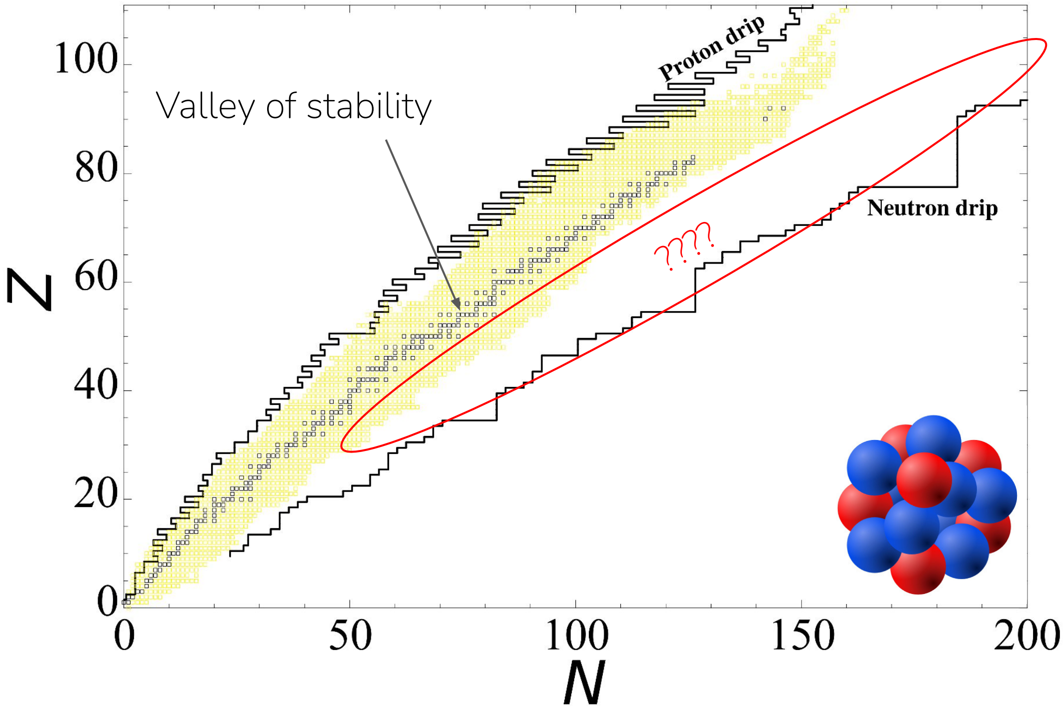


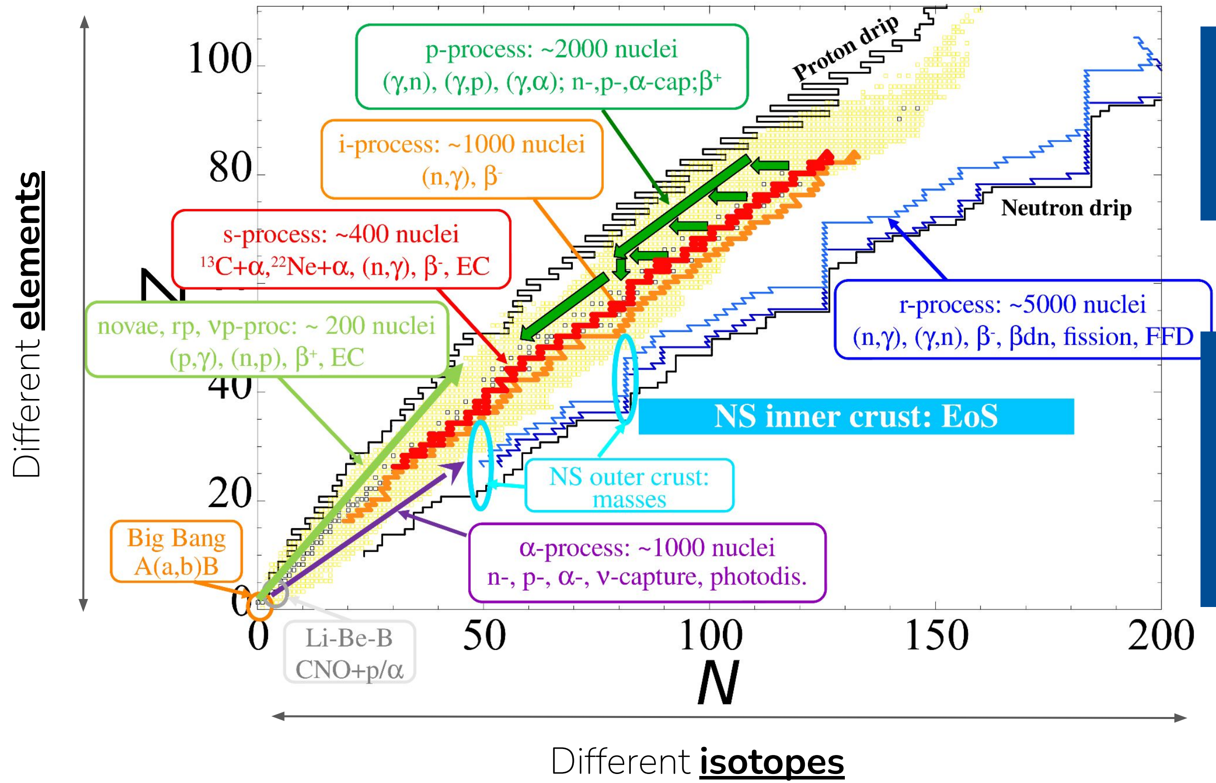

Different **isotopes**

## Transmutation

1. neutron capture
2. β+ and β- decay
3. different types of fission

and many others…

# The nuclear chart and the processes traversing it




## Transmutation

1. neutron capture
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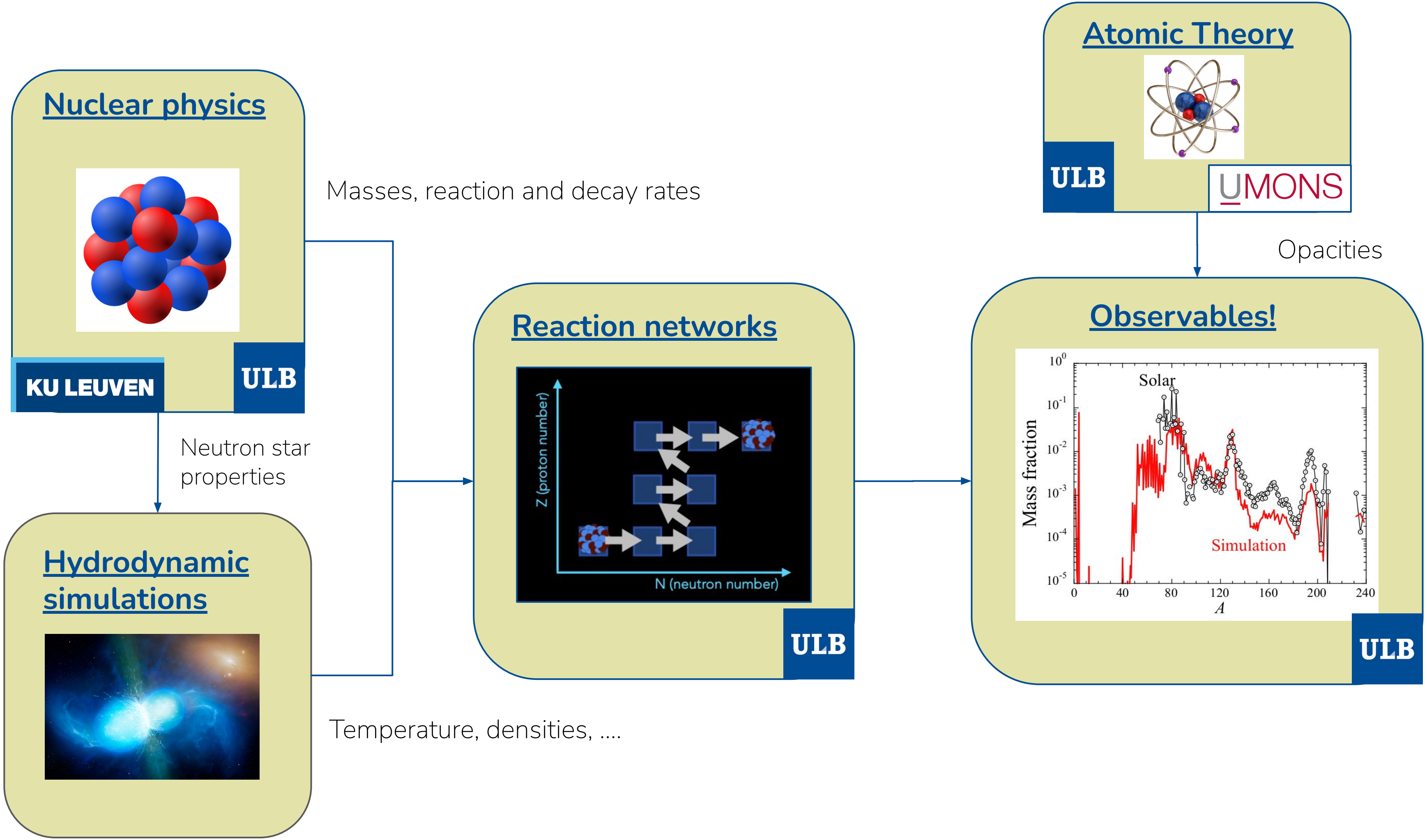
and many others...

## Need for theory!

1. many astrophysical processes
   - r-process, s-process, ...
2. operating in different conditions
   - temperature, density, ...
3. properties of 1000s of nuclei
   - masses, sizes, ...
   - reaction rates



Nuclear physics
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Masses, reaction and decay rates
Neutron star
properties
Hydrodynamic
simulations
Temperature, densities, ....
Reaction networks
Z (proton number)
N (neutron number)
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Atomic Theory
ULB
UMONS
Opacities
Observables!
Solar
Simulation
Mass fraction
A
ULB

# Simulating **one** nucleus

Parameters (N~25)

$$E \sim \int d^3 r \left[ C^\rho \rho(\mathbf{r})\rho(\mathbf{r}) + C^\tau \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

Energy ~ mass

Nuclear densities

**The nuclear many-body problem**

- quantum N-body problem
- … for A~10 - 300 particles
- … with Coulomb interaction
- … with strong nuclear interaction

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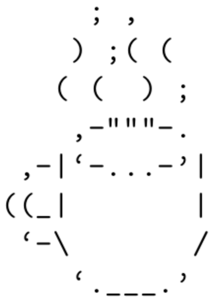

### The nuclear many-body problem

- quantum N-body problem
- … for A~10 - 300 particles
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- … with strong nuclear interaction

### Density Functional Theory with MOCCa

- non-linear optimisation problem

# Simulating **one** nucleus

Typical job: 0.3-1h, $<$ 2GB, 1 CPU
Extreme job: 6 - 7h , ~ 4GB, 1 CPU
On LUMI: ?

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$$E \sim \int d^3r \left[ C^{\rho} \rho(\mathbf{r})\rho(\mathbf{r}) + C^{\tau} \tau(\mathbf{r})\rho(\mathbf{r}) + \dots \right]$$

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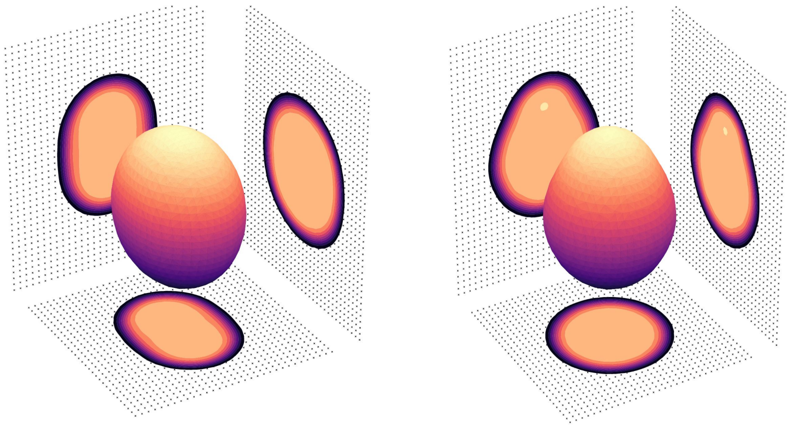

## The nuclear many-body problem

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## Nuclear Density Functional Theory

- non-linear optimisation problem
- 3D coordinate space representation
- need to explore different shapes

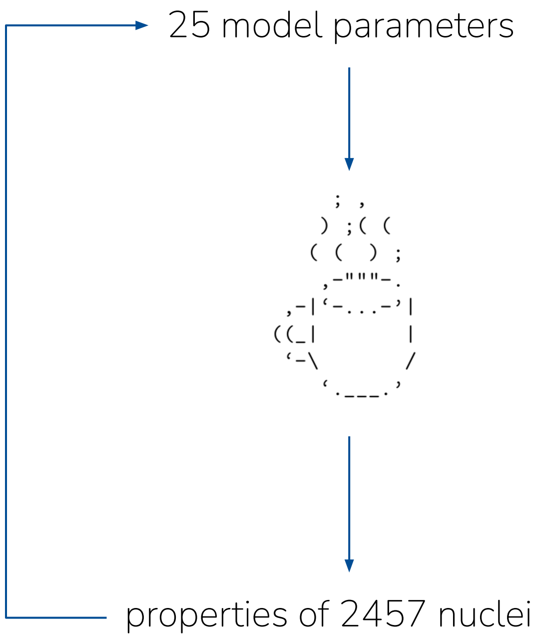
# Simulating **7000** nuclei: building models

Fit to experimental data:

- 2457 nuclear masses
- 884 charge radii
- 45 fission barriers

Optimisation problem:

- high-dimensional
- function evaluation ex. costly
- highly non-linear



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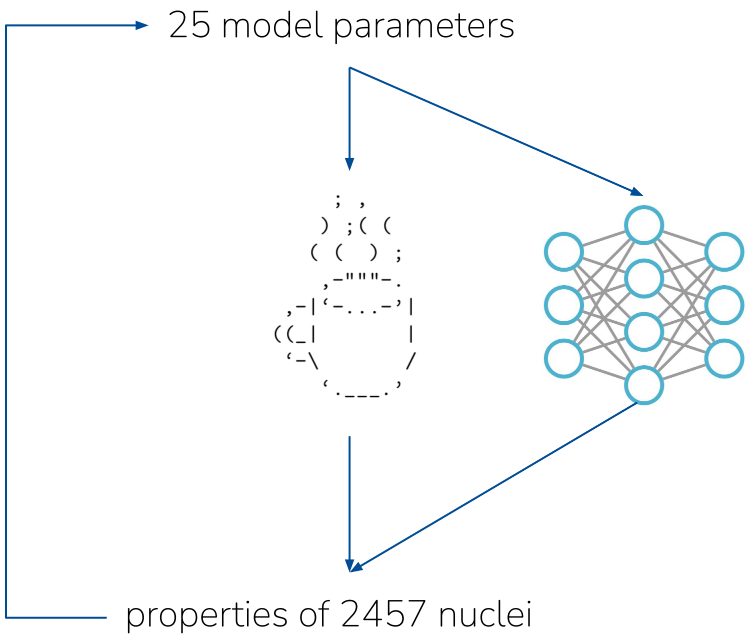
- committee of neural networks
- each emulates MOCCa
- efficient exploration of parameter space



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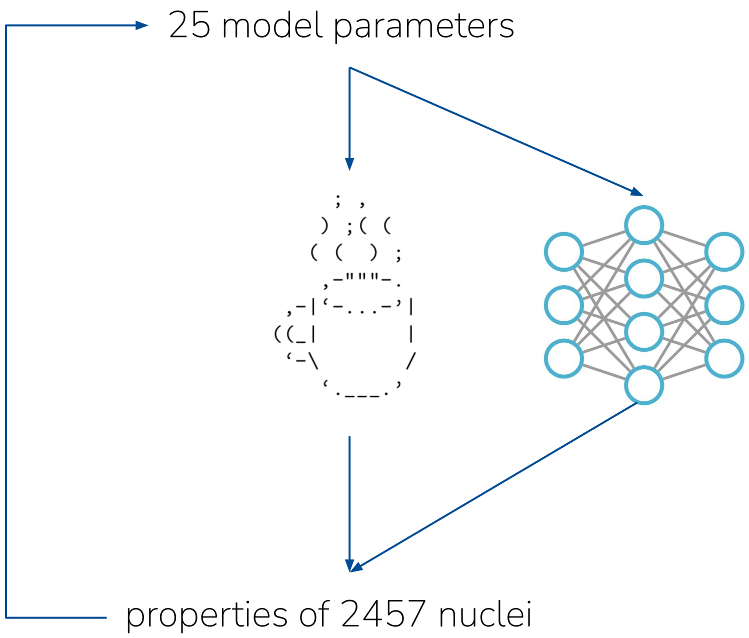
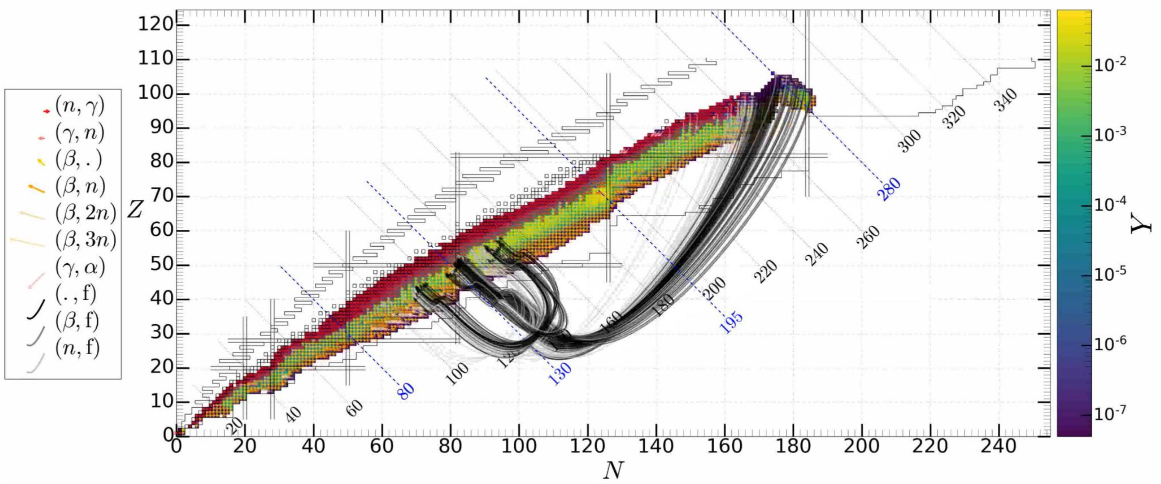
**BSkG3: 1.5 years of development, ~2x10$^6$ CPU hours!**



# Reaction networks

Typical job: 4 days, ~ 1GB, 1 CPU




**One “trajectory”**

- ~ 5000 stiff, coupled, first-order ODEs
- one set of astrophysical conditions
- variable runtime

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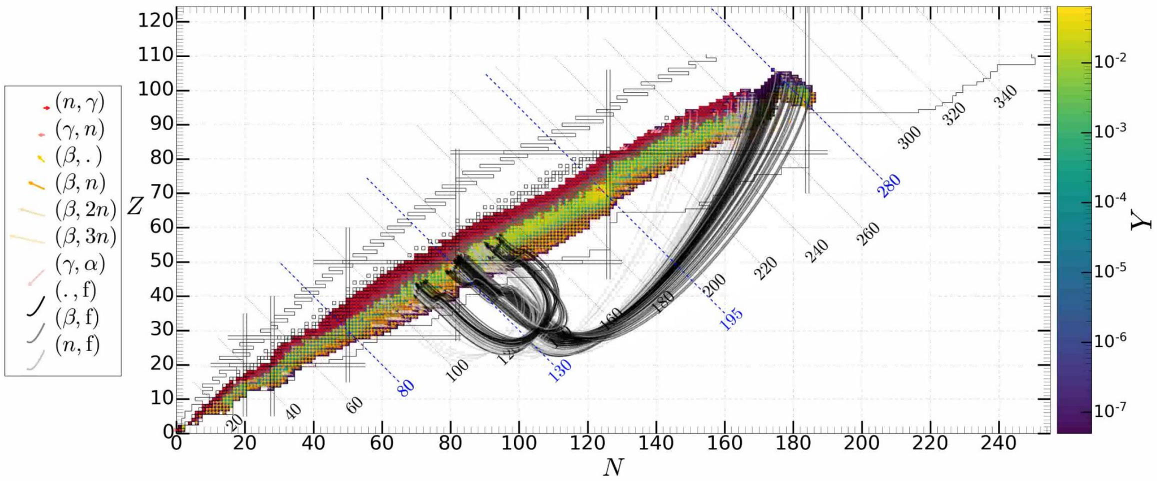



**One "trajectory"**

- ~ 5000 stiff, coupled, first-order ODEs
- one set of astrophysical conditions
- variable runtime

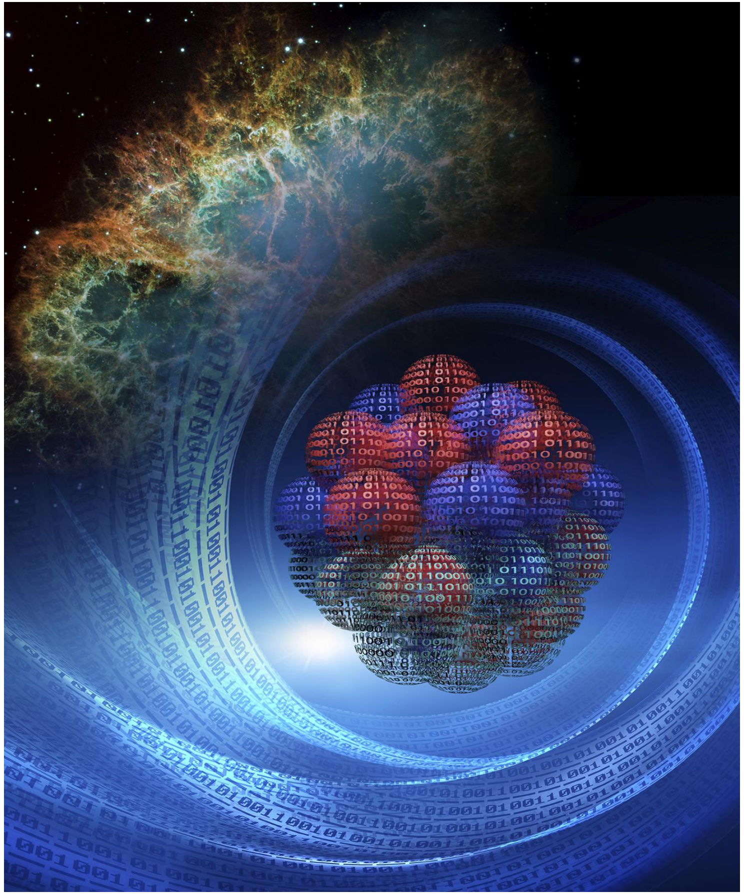
**Realistic simulations ~ 1k-2k trajectories**

- different colliding stars
- ejecta with different temperatures/densities
- uncertainty study of nuclear models

# Conclusion

From the **microscopic** description of **nuclei**
and their **many** properties

- non-linear optimisation problem with 3D geometries
- large-scale parameter adjustments with neural networks
- large-scale calculations for the extraction of reaction rates



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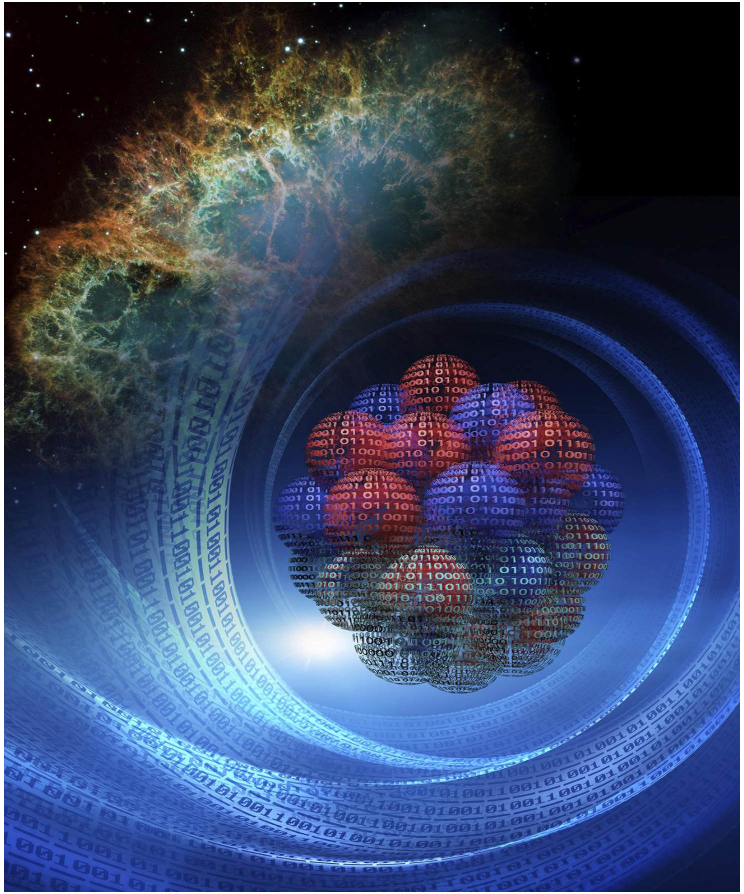
.... to the **macroscopic** explosion of **stars** ....

- large reaction-network calculations
- ..... for different thermodynamic conditions
- .... for different nuclear models



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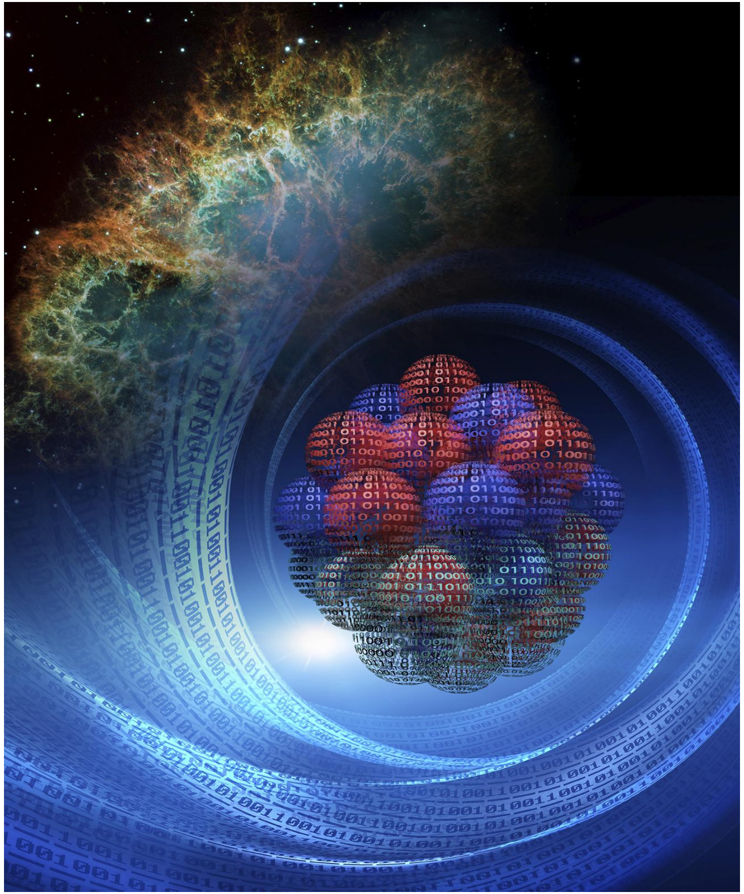
... to find out where the **elements** come from!



# Thank you ....

...... to all our Belgian collaborators!

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...and the patient user support!

Cenaero

CÉCI

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...... for your attention!