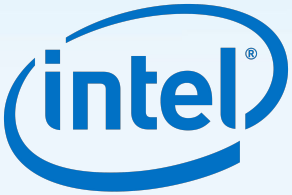
Magritte

A **modern** software library for **3D radiative transfer**

Frederik De Ceuster

in collaboration with

Ward Homan, Jeremy Yates, Leen Decin,
James Hetherington, Guido Cossu, Peter Boyle, ...



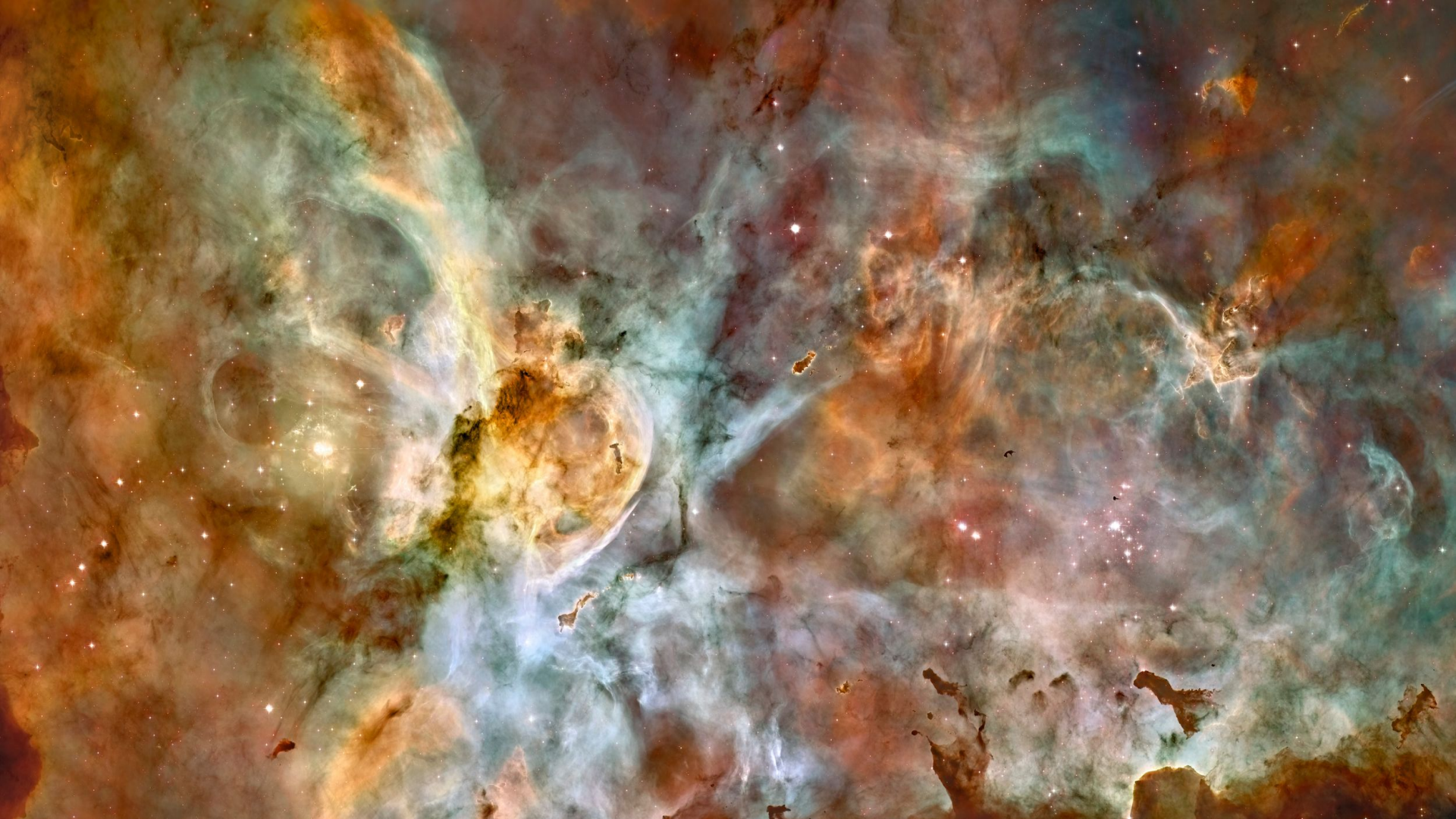
EPSRC iCASE studentship

Training Programme

Solving **Radiative Transfer** problems using **Math** and **Technology**

Solving **Radiative Transfer** problems

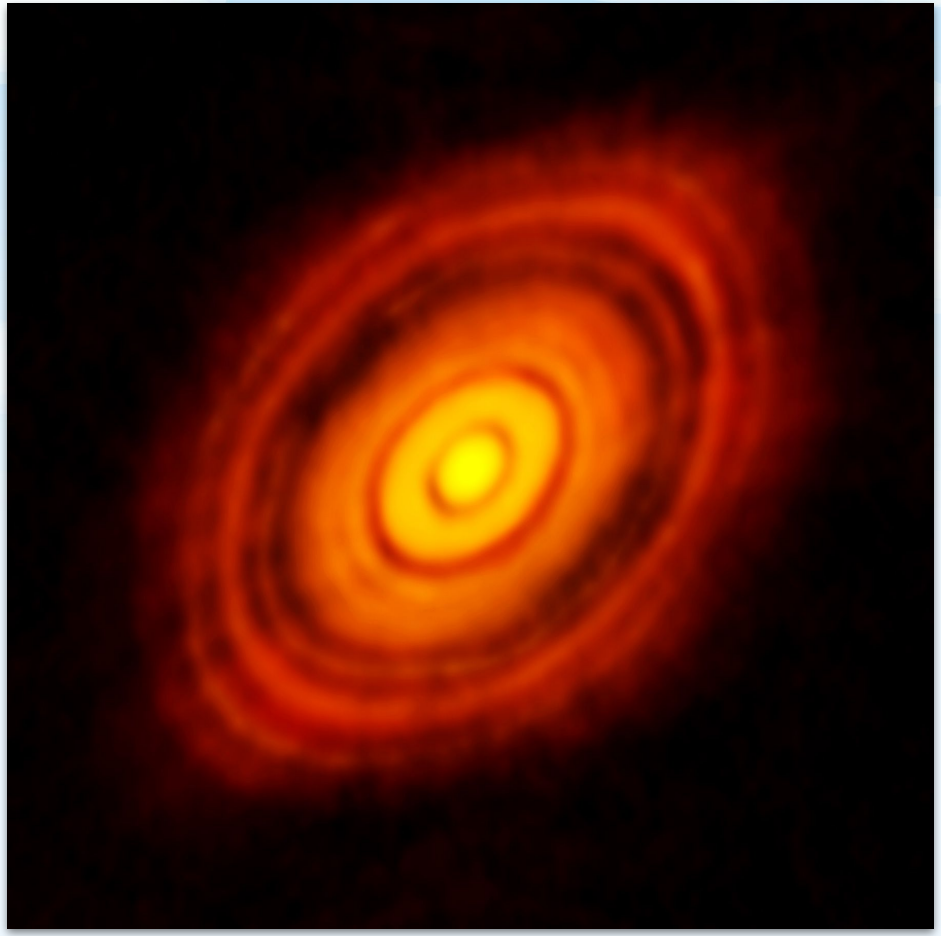
using **Math** and **Technology**



Atacama
Large
Millimetre
Array

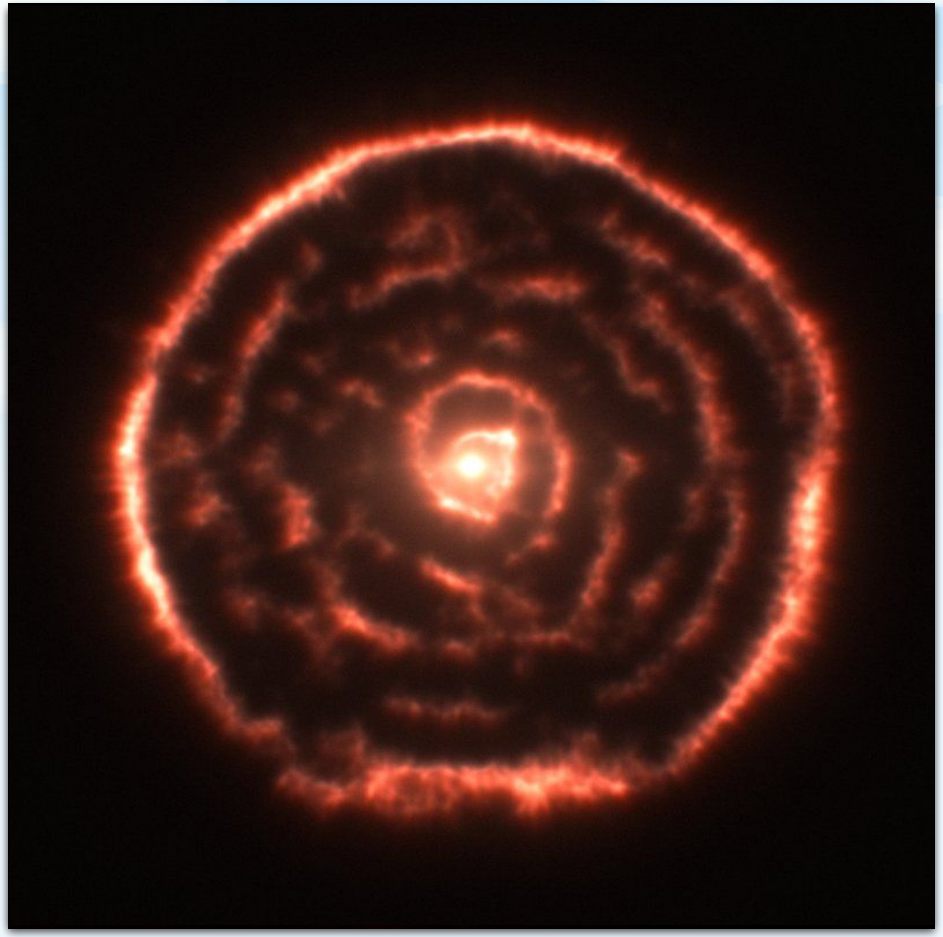
Disk HL Tauri

(ALMA et al. 2015)



Spiral R Sculptoris

(Maercker et al. 2012)



Understanding physics and chemistry

through computational **modelling**

Magritte's Radiative Transfer solver

Most Radiative Transfer solvers

Most Radiative Transfer solvers: Monte Carlo

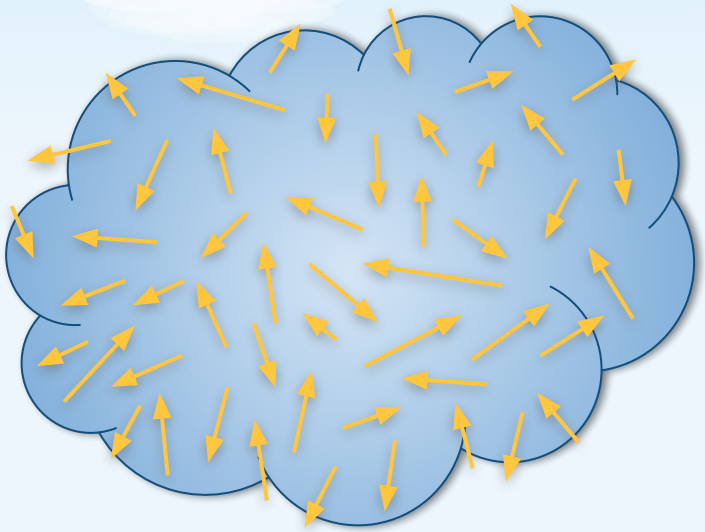
*"**Propagate** photon packets through the medium"*

Noebauer & Sim (2019)

(+) Fast & Intuitive

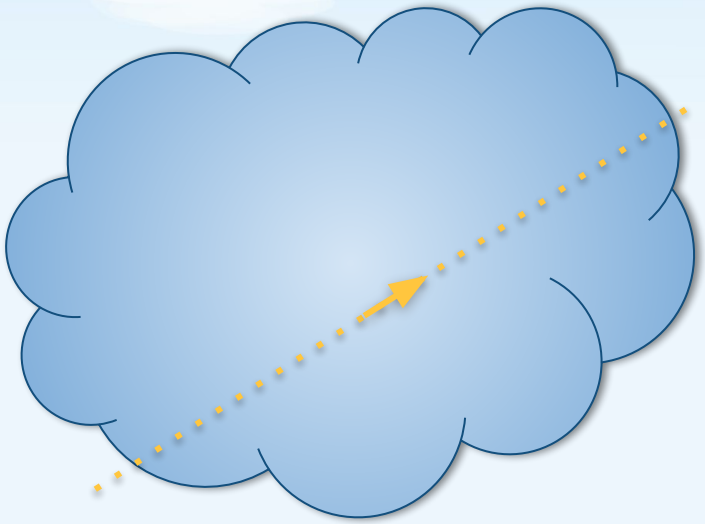
(–) Photon trapping

Camps & Baes (2018)



Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*



Magritte's Radiative Transfer solver

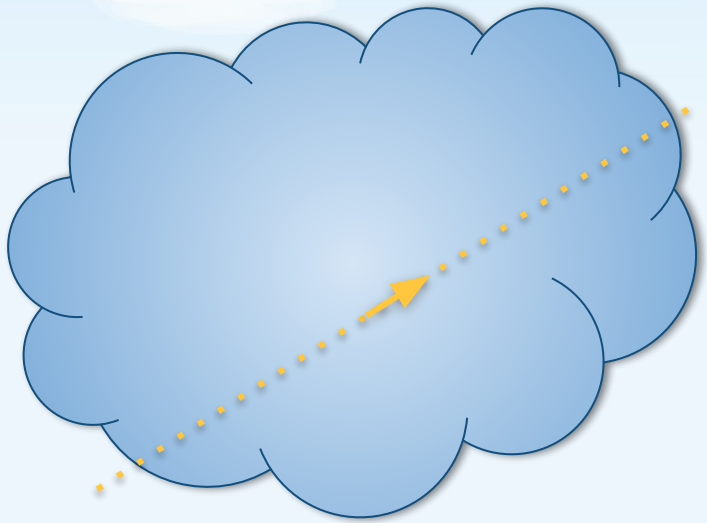
*"**Solve** the radiative transfer equation **along a ray**"*

What is a ray?

Straight line through the model

How to trace a ray?

...



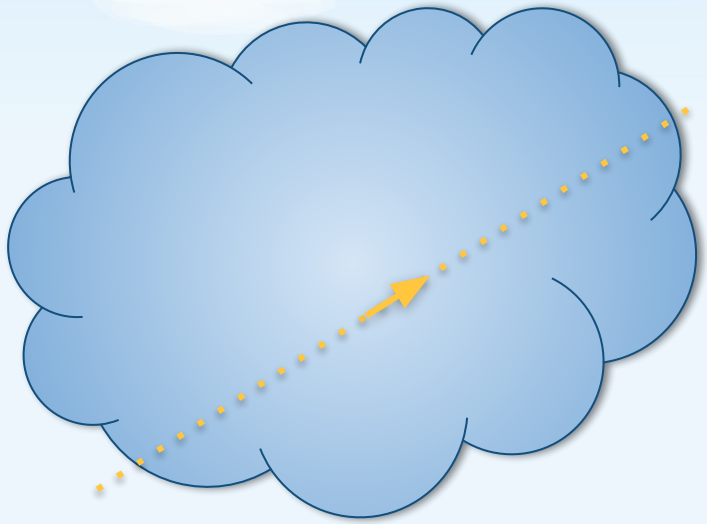
Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*

$$\frac{\mathrm{d}I}{\mathrm{d}z} = \eta - \chi I$$

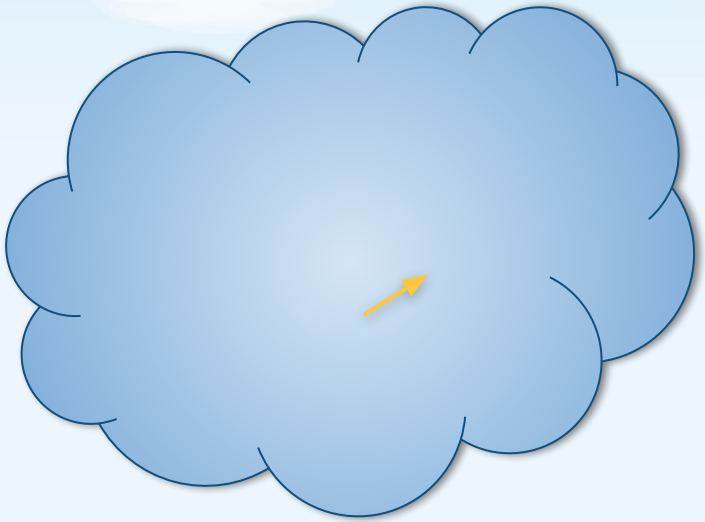
$\eta =$ emissivity

$\chi =$ opacity



Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*



Magritte's Radiative Transfer solver

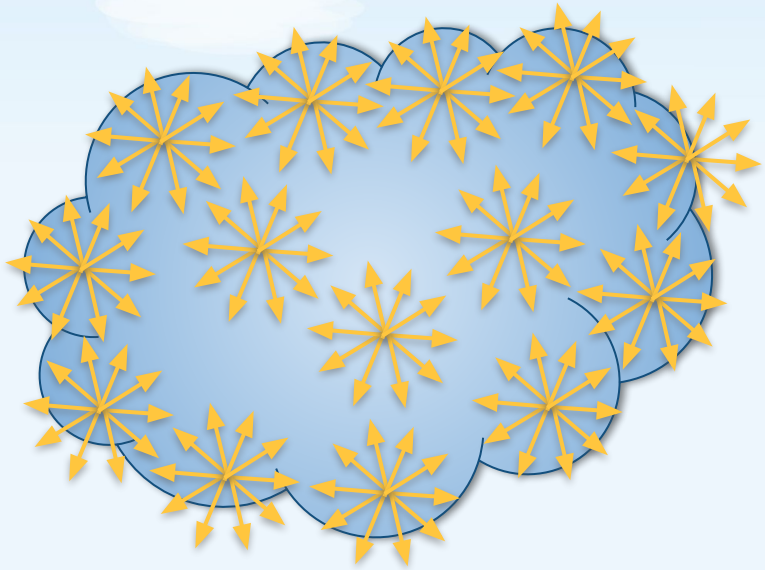
*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction***

Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*

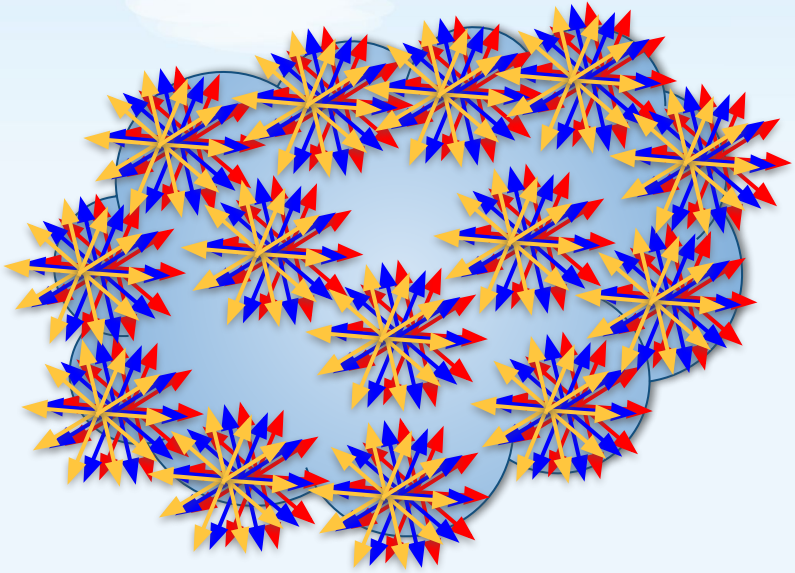
- *for each **direction***
- *for each **point***



Magritte's Radiative Transfer solver

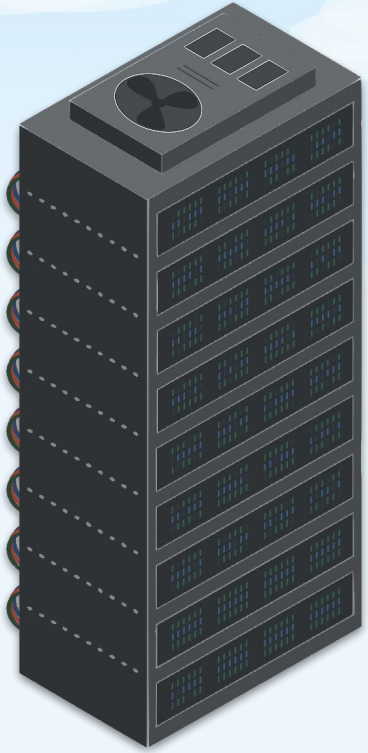
*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction***
- *for each **point***
- *for each **frequency bin***



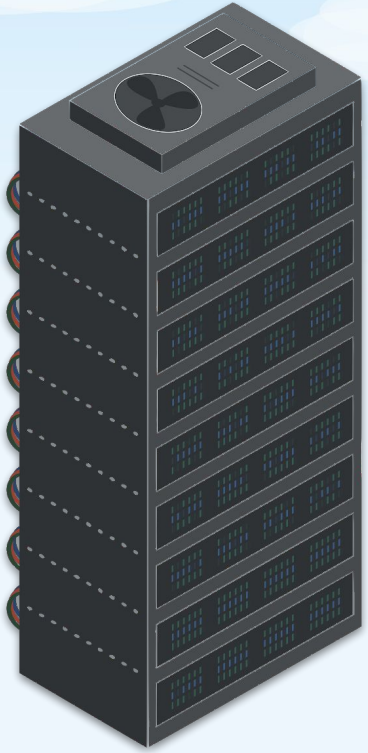
Technology to the rescue!

Modern high-performance architecture



- Layers of **parallelism**
- Hardware **accelerators**

Modern high-performance architecture

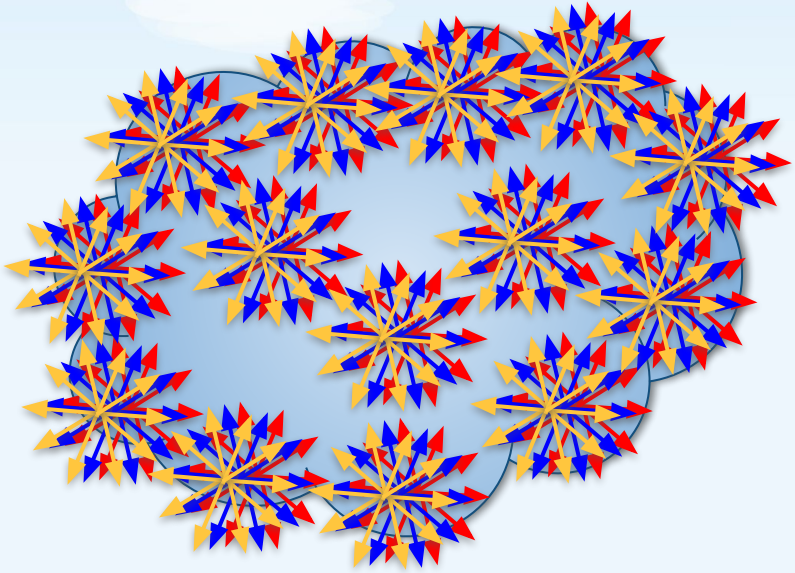


- Layers of **parallelism**
- Hardware **accelerators**

Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction***
- *for each **point***
- *for each **frequency bin***

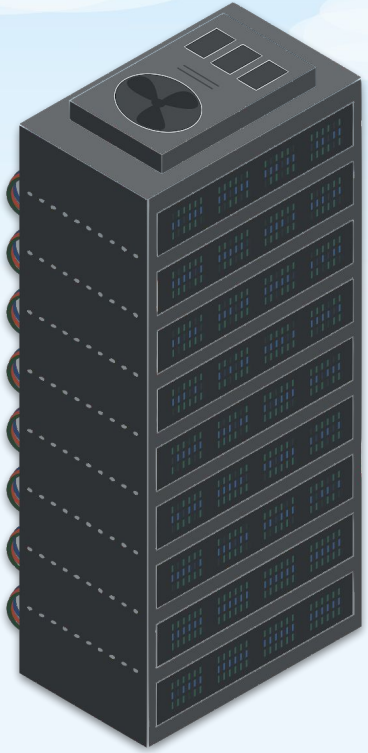


Magritte's Radiative Transfer solver

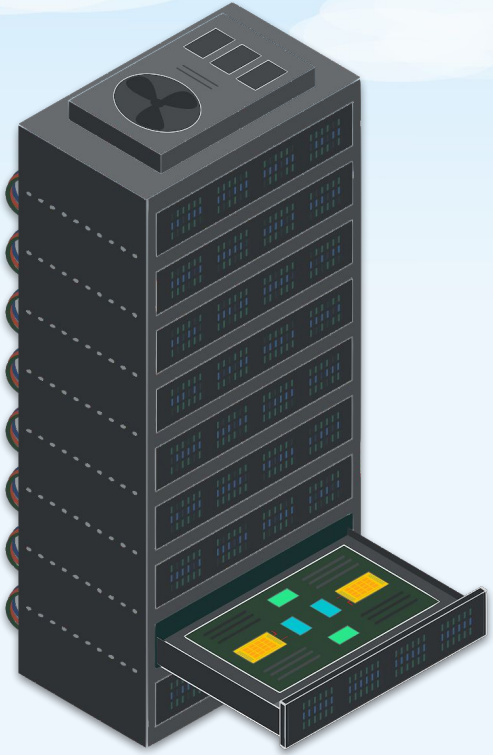
*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction*** nodes (MPI)
- *for each **point*** cores / threads (OpenMP)
- *for each **frequency bin*** vectorisation (Grid-SIMD)

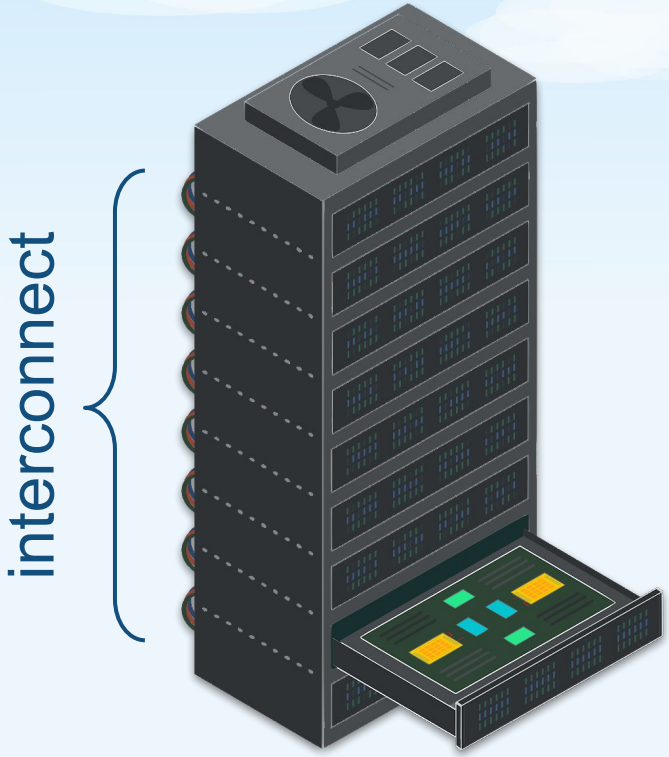
Modern high-performance architecture



Modern high-performance architecture



Modern high-performance architecture



Node-level parallelism


COMPUTING
DIVISION
COMPUTING
SECTION

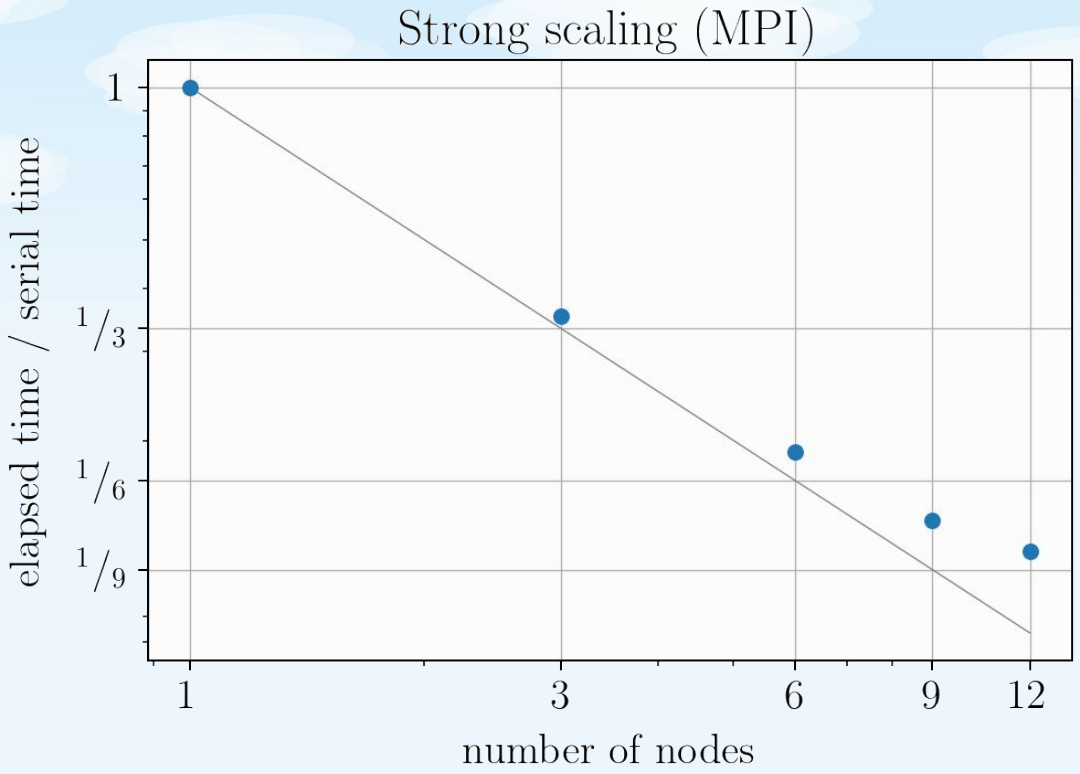
- **Distributed** memory
- Communication via **message passing** (MPI)
- Relatively **slow**

Magritte's Radiative Transfer solver

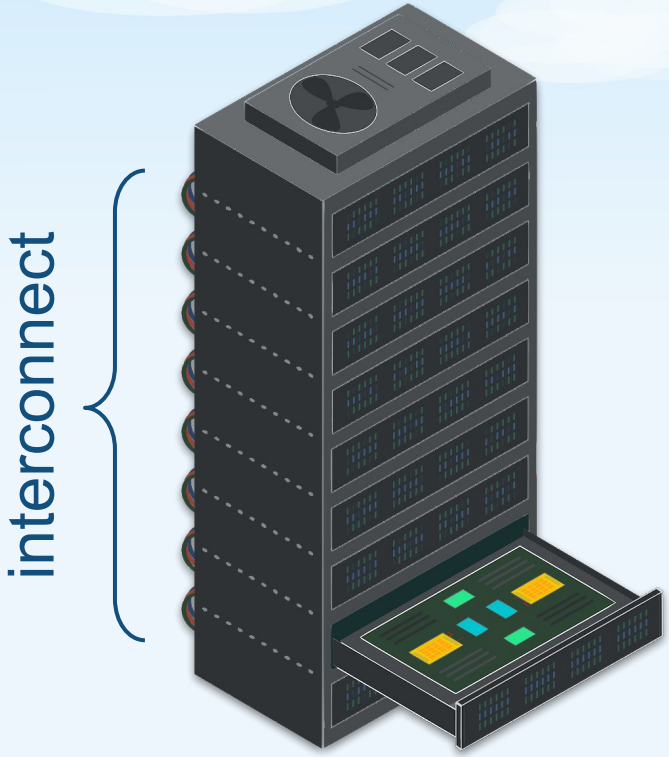
*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction*** nodes (MPI)
- *for each **point*** cores / threads (OpenMP)
- *for each **frequency bin*** vectorisation (Grid-SIMD)

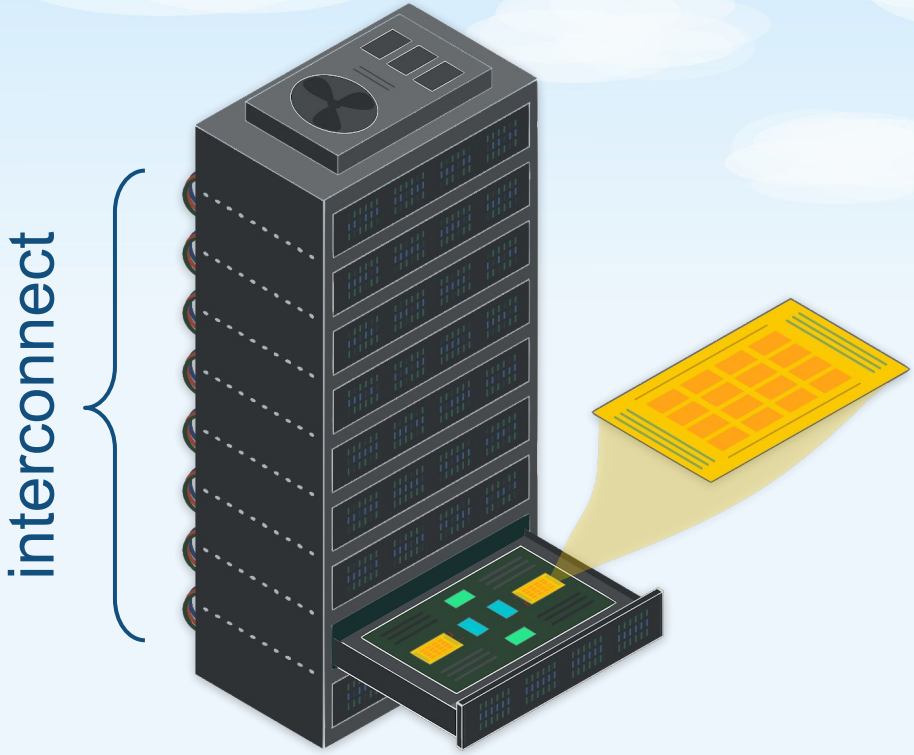
Magritte's MPI parallelisation



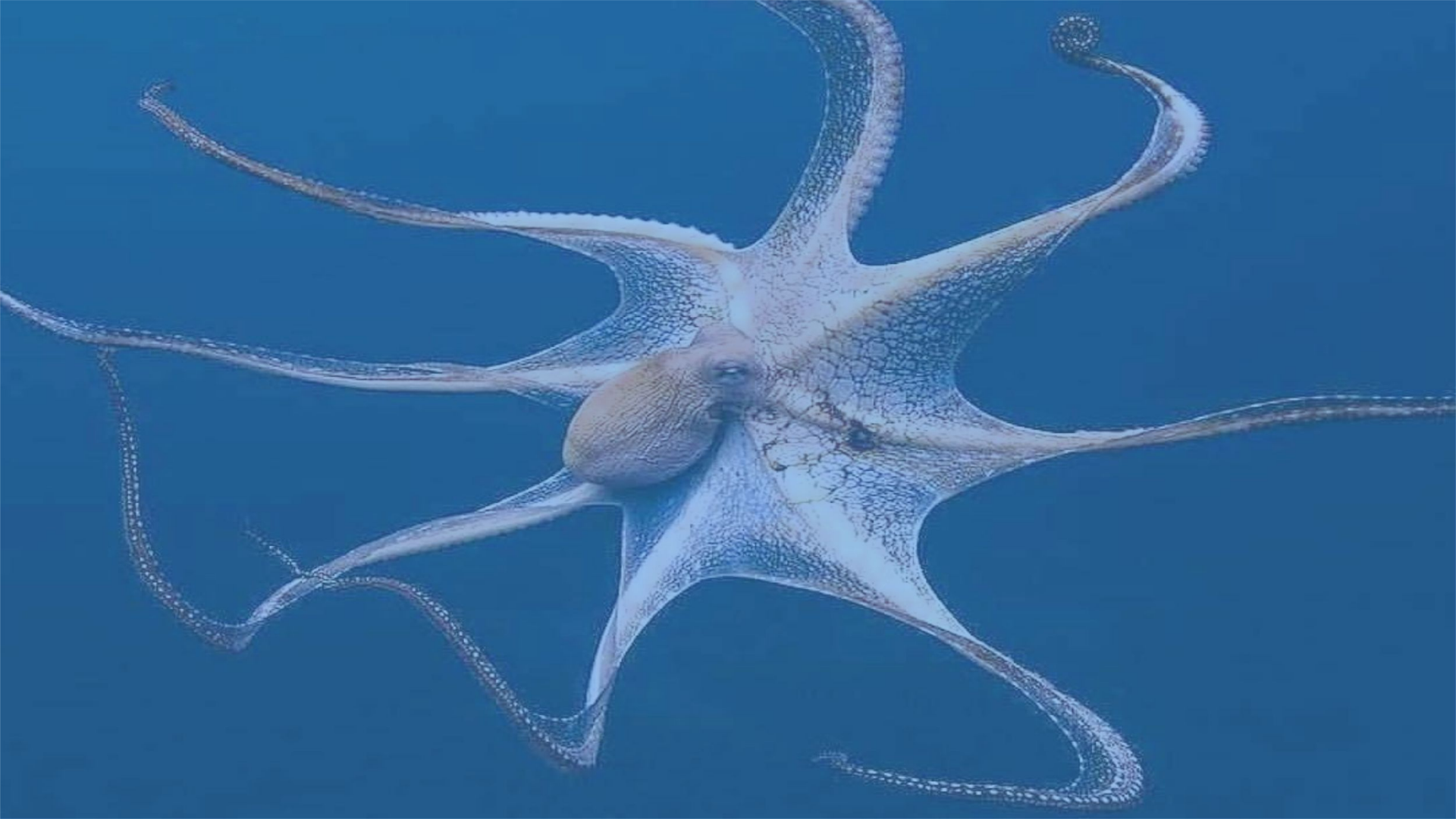
Modern high-performance architecture

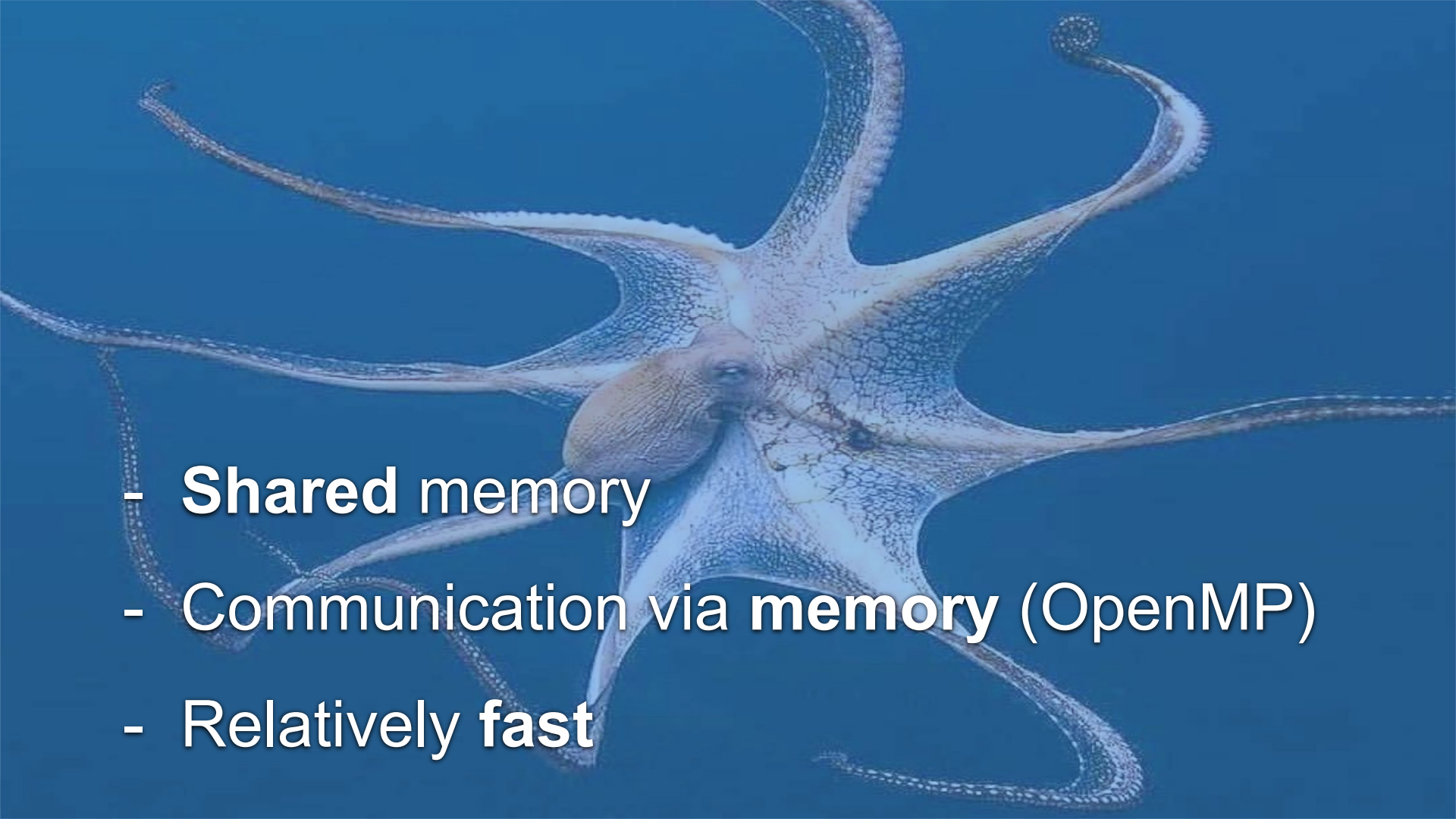


Modern high-performance architecture




Thread-level
parallelism





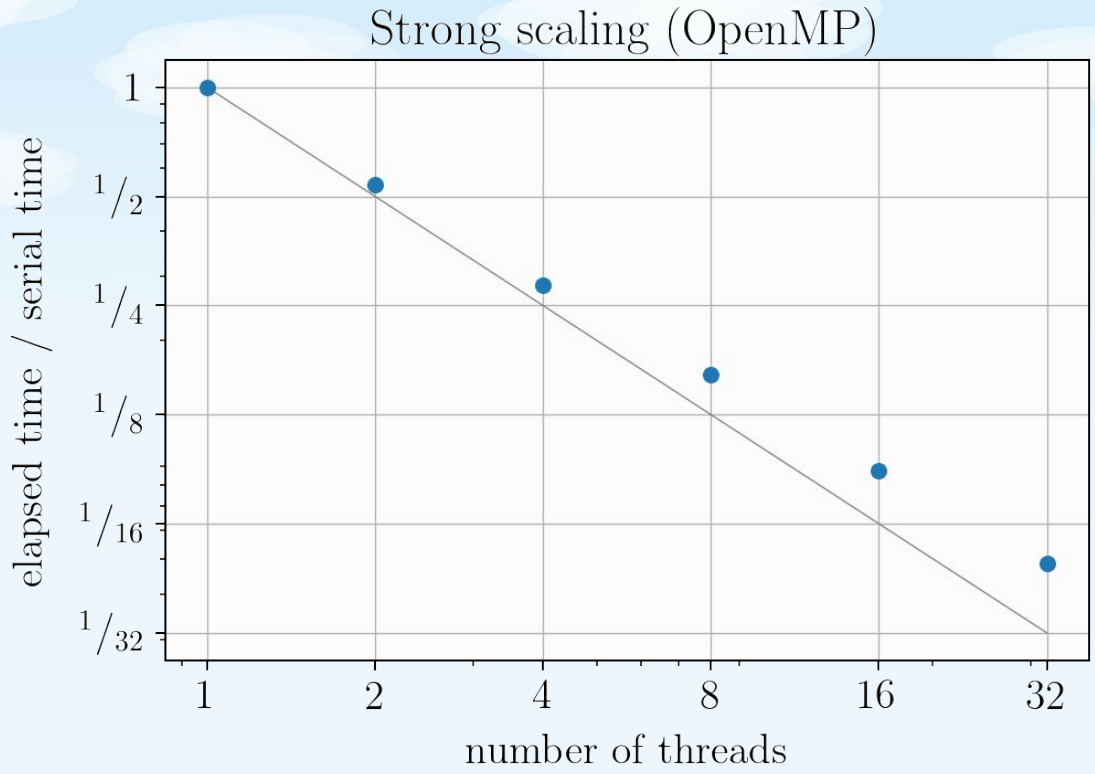
- **Shared** memory
- Communication via **memory** (OpenMP)
- Relatively **fast**

Magritte's Radiative Transfer solver

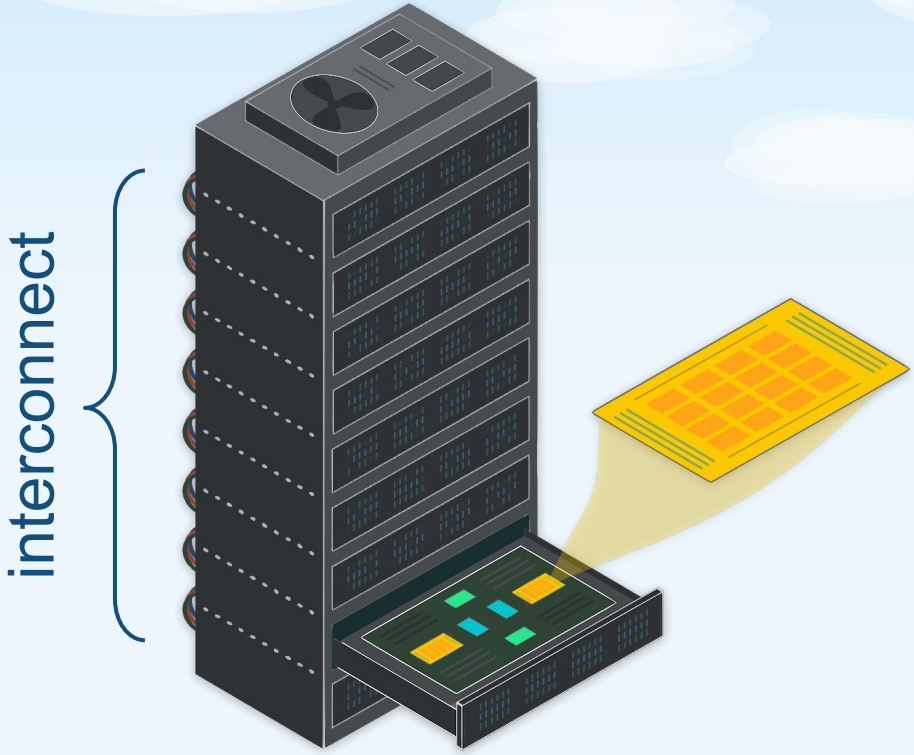
*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction*** nodes (MPI)
- *for each **point*** cores / threads (OpenMP)
- *for each **frequency bin*** vectorisation (Grid-SIMD)

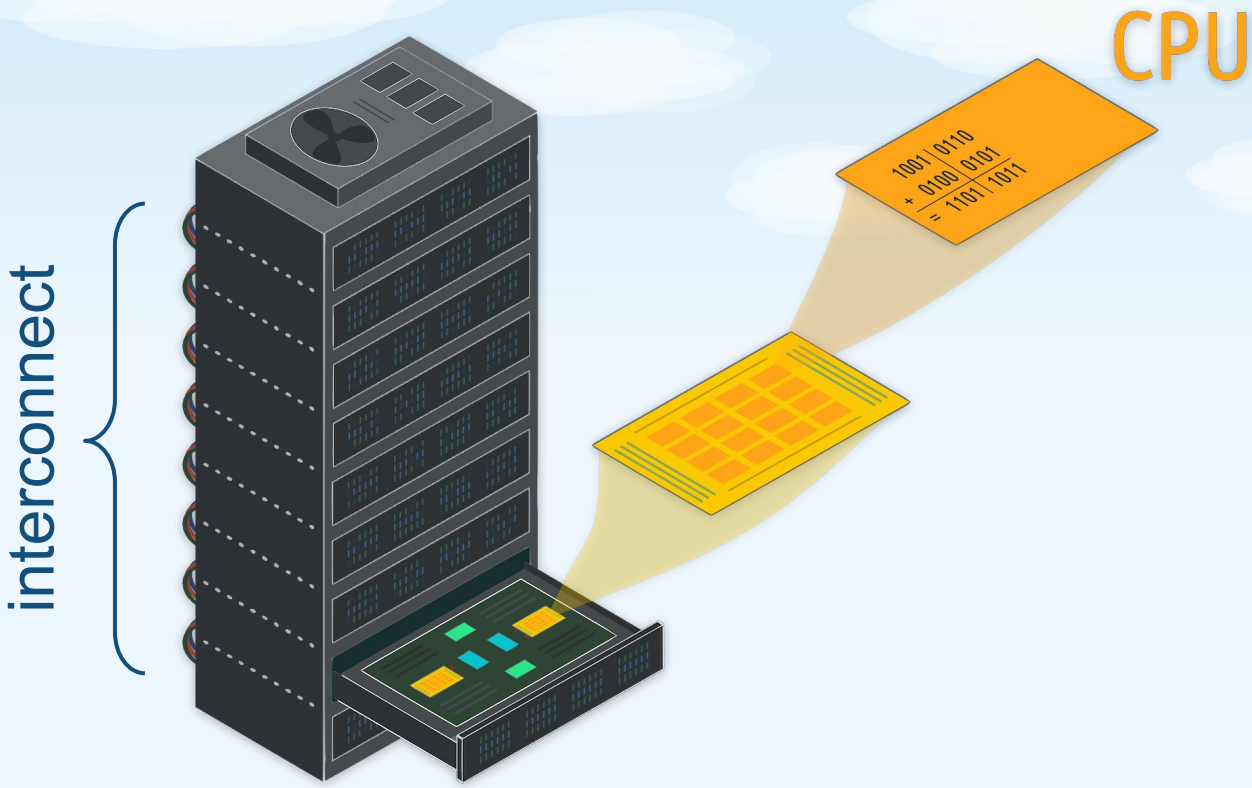
Magritte's OpenMP parallelisation



Modern high-performance architecture



Modern high-performance architecture




Vectorisation


SIMD-parallelism

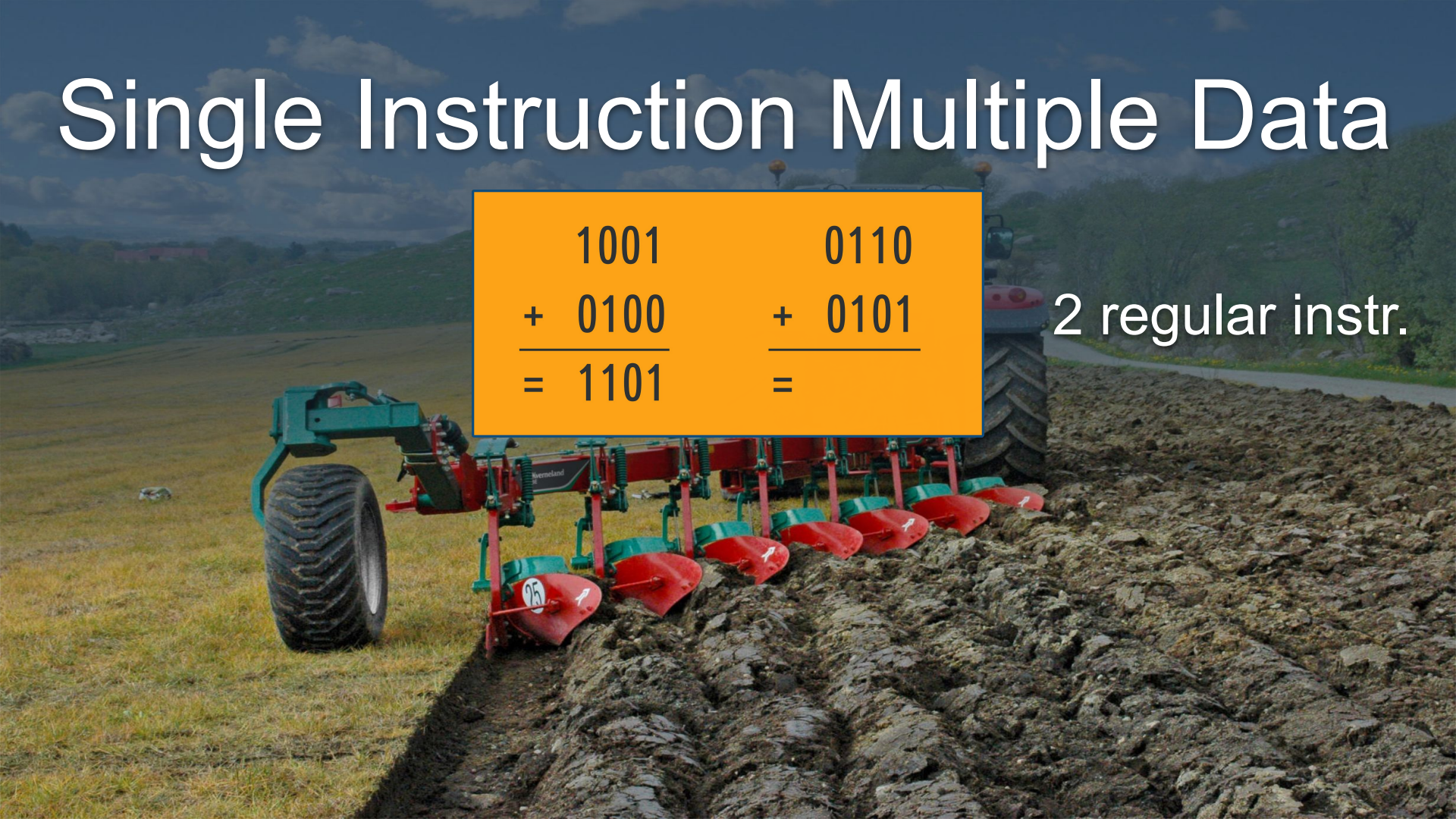
Single Instruction Multiple Data

Single Instruction Multiple Data

1001	0110
+ 0100	+ 0101
=	=

2 regular instr.

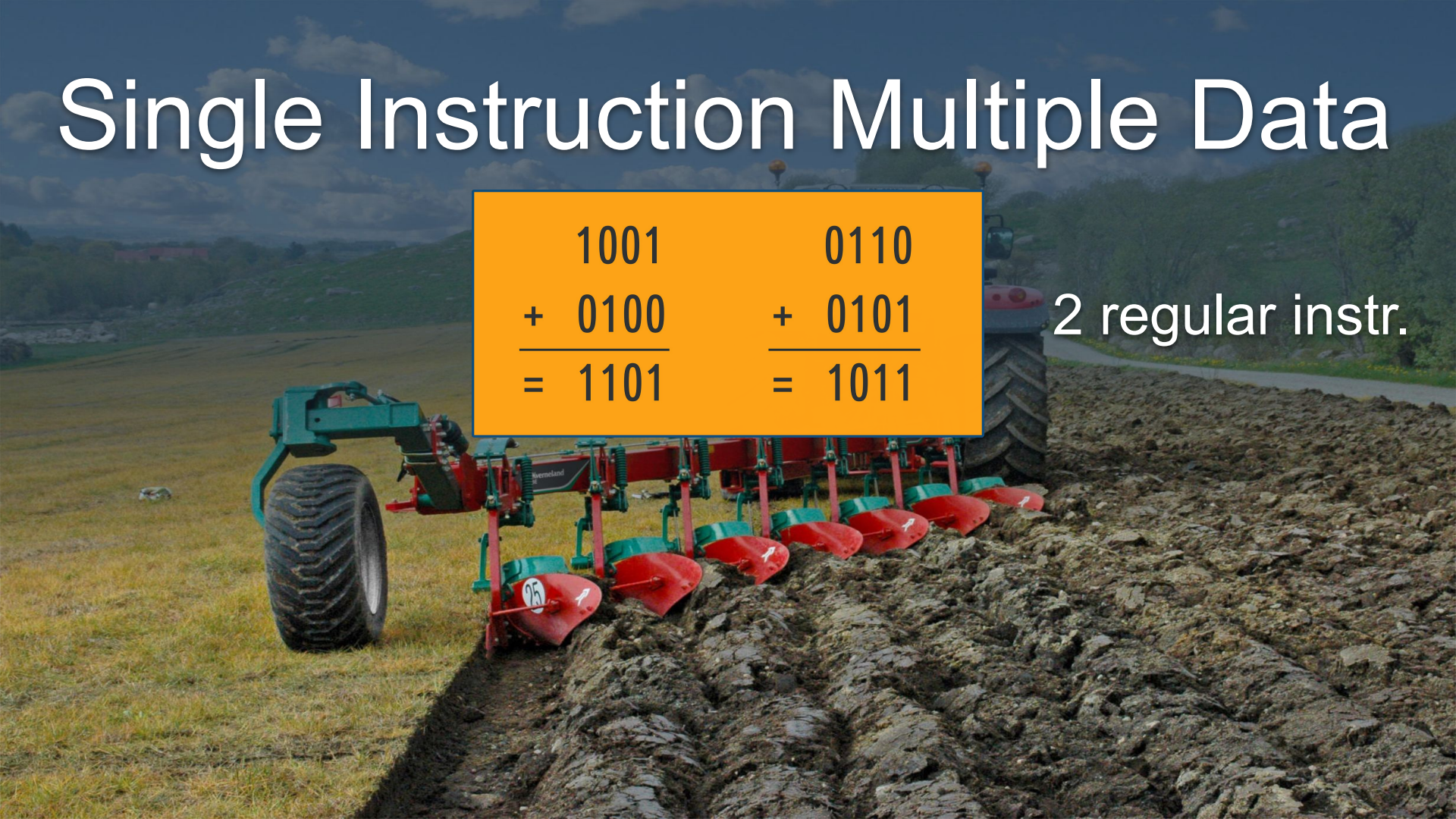
Single Instruction Multiple Data



1001	0110
+ 0100	+ 0101
= 1101	=

2 regular instr.

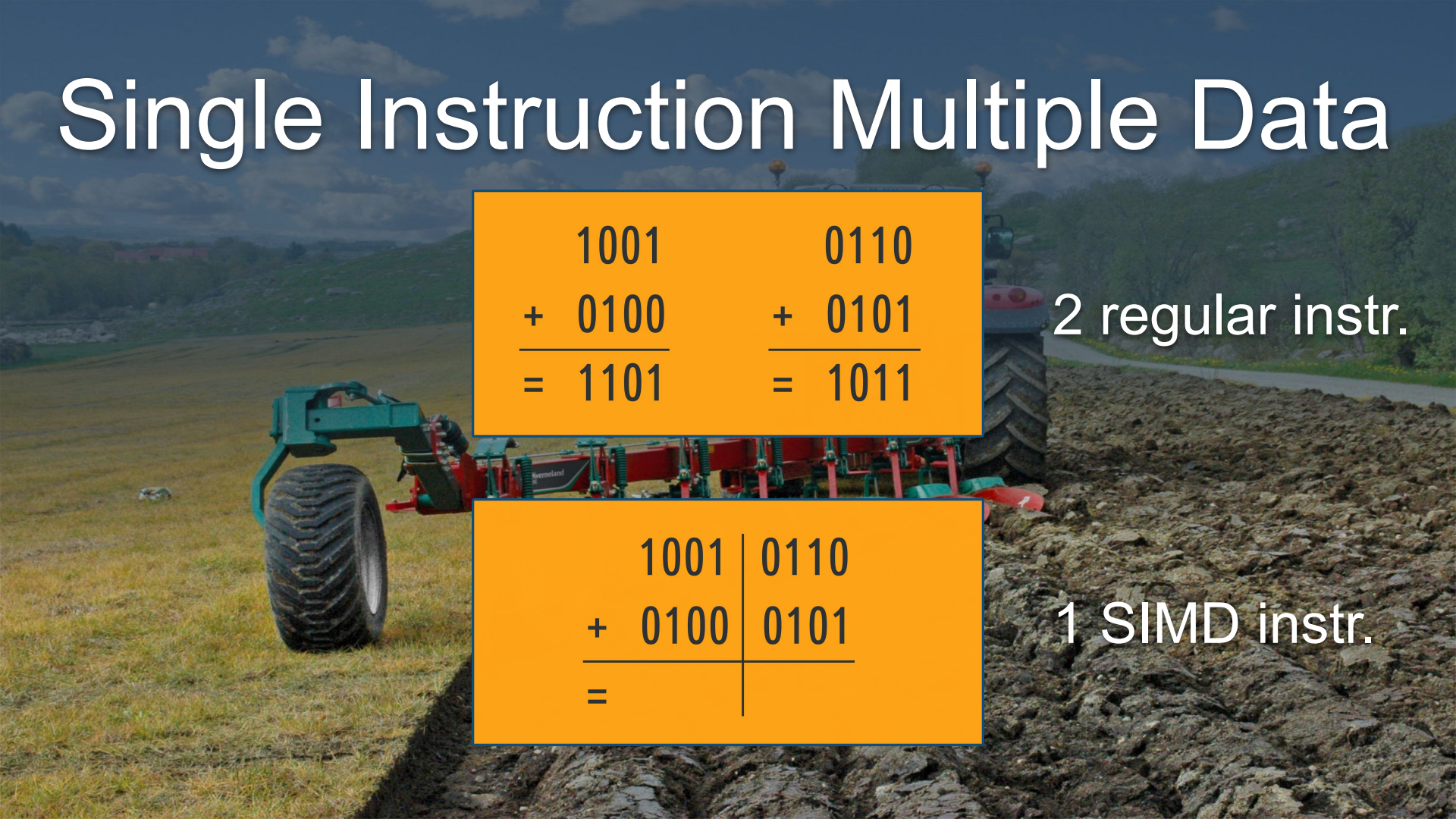
Single Instruction Multiple Data



1001	0110
+ 0100	+ 0101
= 1101	= 1011

2 regular instr.

Single Instruction Multiple Data



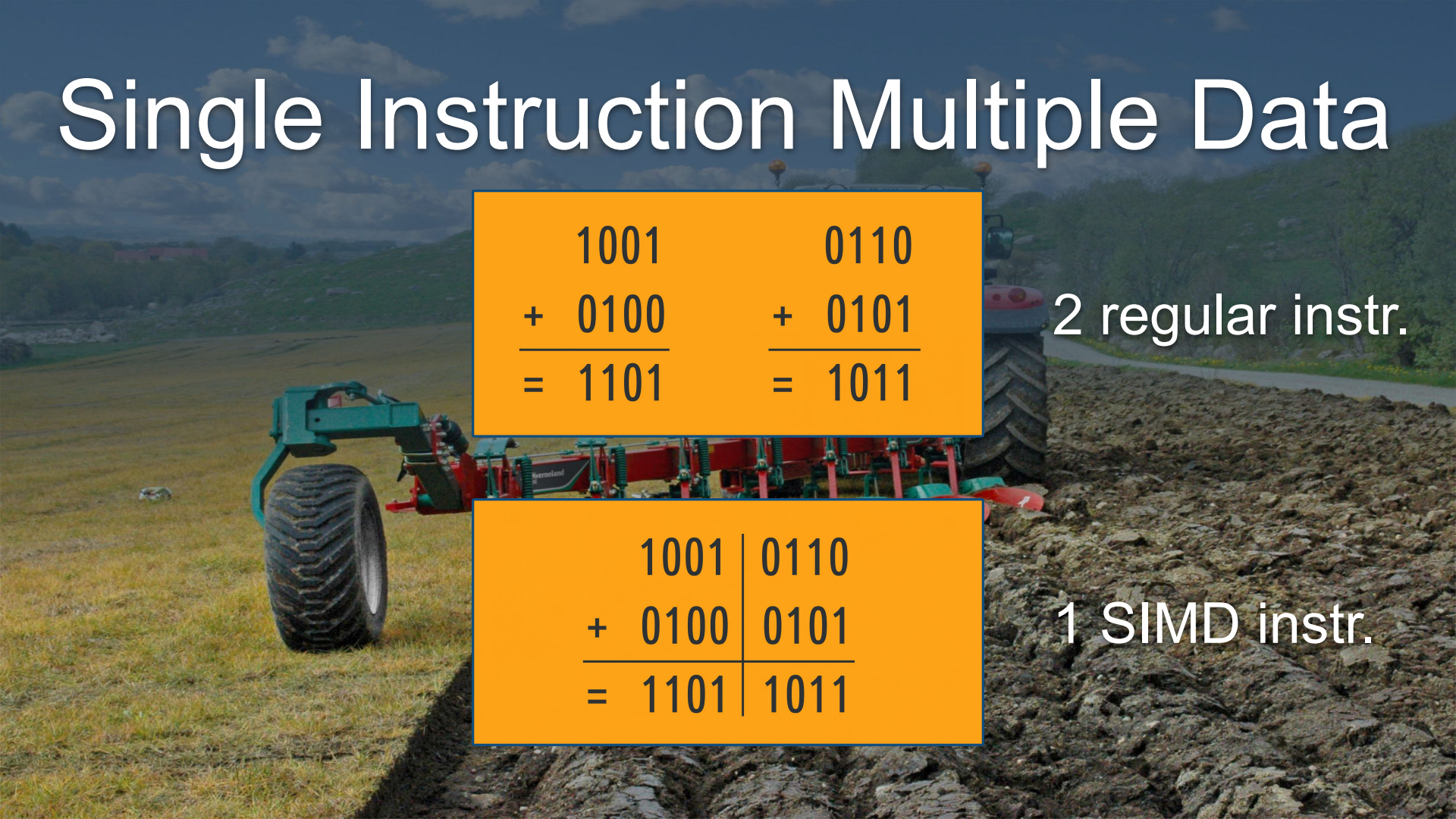
1001	0110
+ 0100	+ 0101
= 1101	= 1011

2 regular instr.

1001 | 0110	
+ 0100 | 0101	
=	

1 SIMD instr.

Single Instruction Multiple Data



1001	0110
+ 0100	+ 0101
= 1101	= 1011

2 regular instr.

1001 | 0110	
+ 0100 | 0101	
= 1101 | 1011	

1 SIMD instr.


Overneland
25

Magritte's Radiative Transfer solver

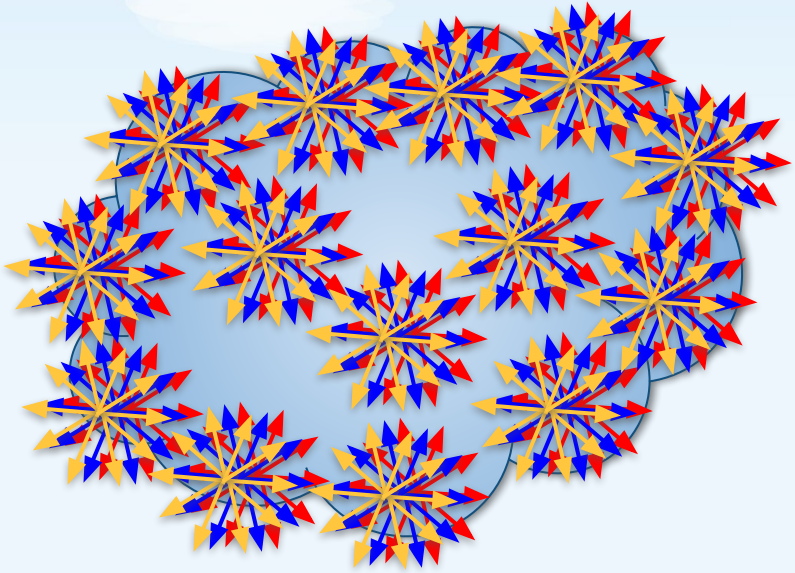
*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction*** nodes (MPI)
- *for each **point*** cores / threads (OpenMP)
- *for each **frequency bin*** vectorisation (Grid-SIMD)

Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*

- *for each **direction***
- *for each **point***
- *for each **frequency bin***

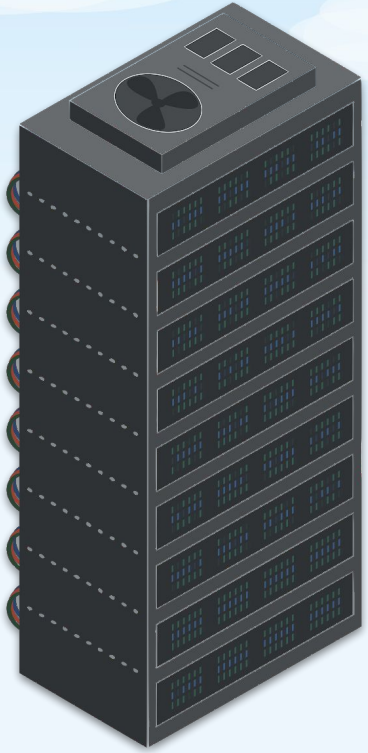


Magritte's Radiative Transfer solver

*"**Solve** the radiative transfer equation **along a ray**"*

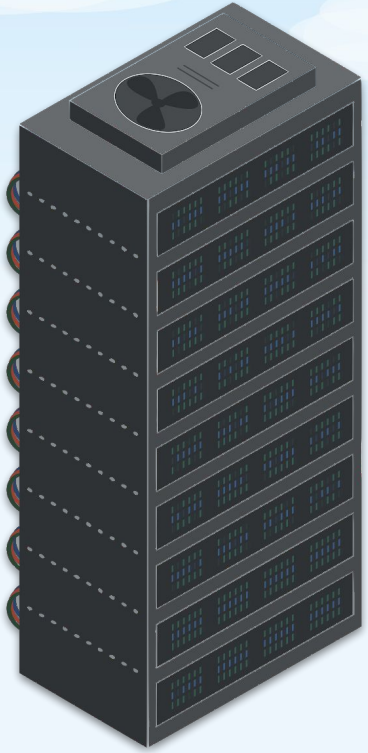
- *for each **direction*** nodes (MPI)
- *for each **point*** cores / threads (OpenMP)
- *for each **frequency bin*** vectorisation (Grid-SIMD)

Modern high-performance architecture



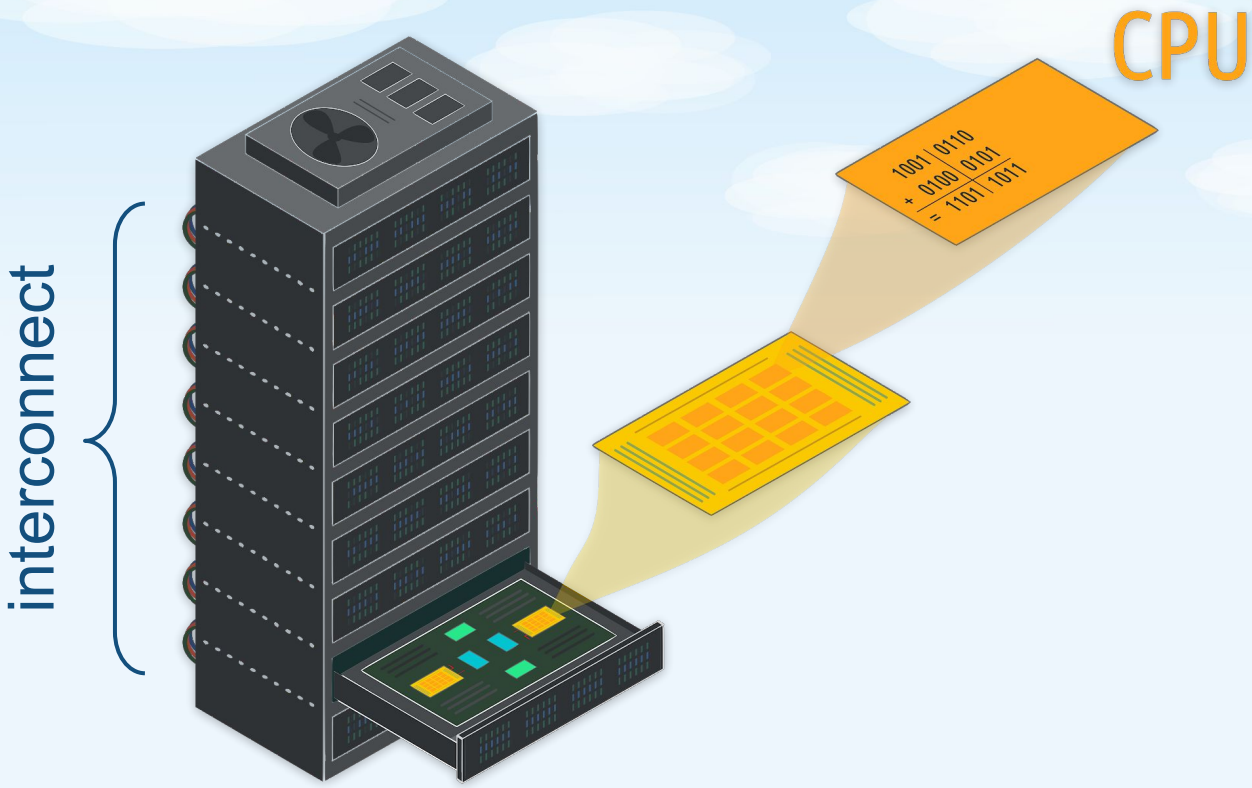
- Layers of **parallelism**
- Hardware **accelerators**

Modern high-performance architecture

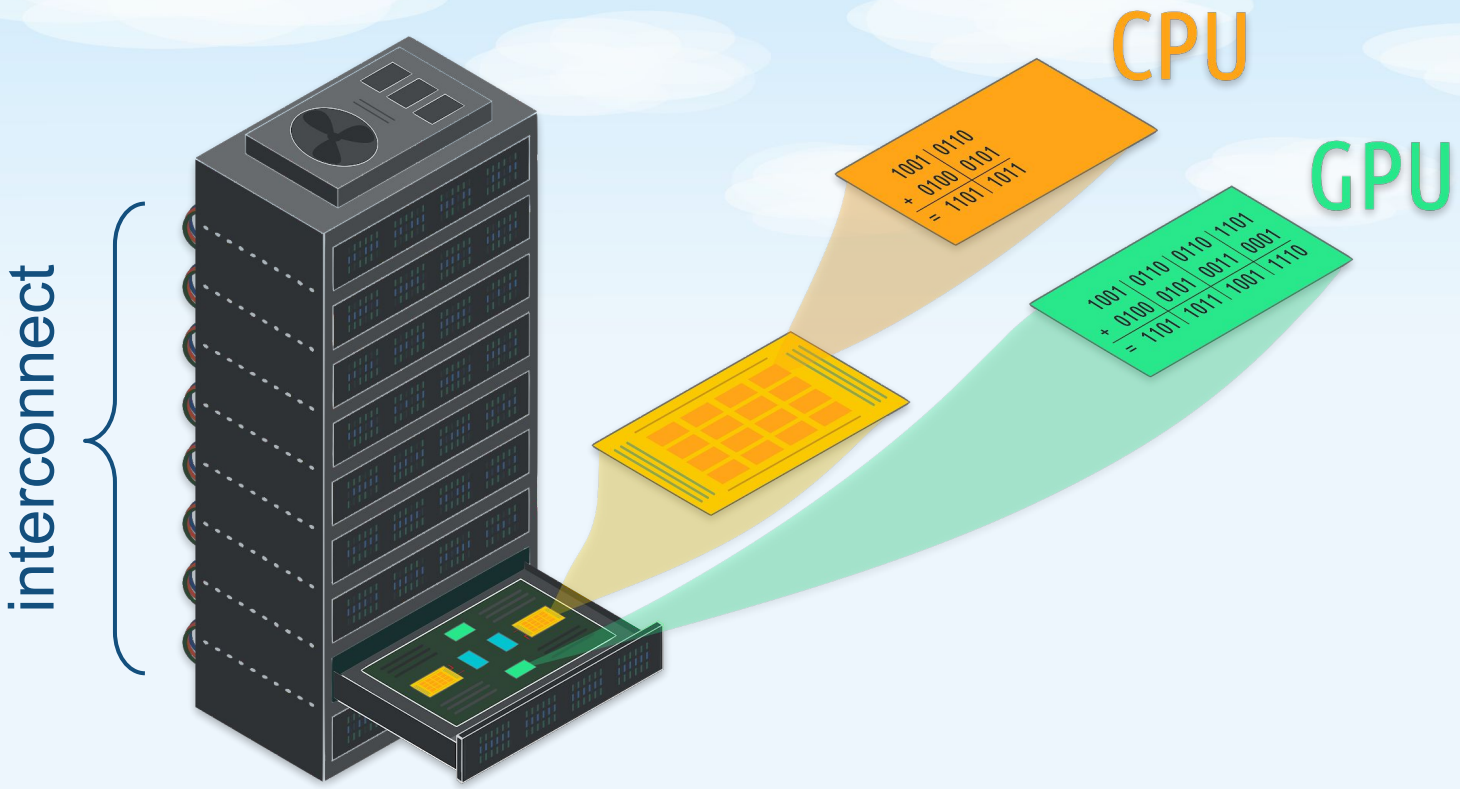


- Layers of **parallelism**
- Hardware **accelerators**

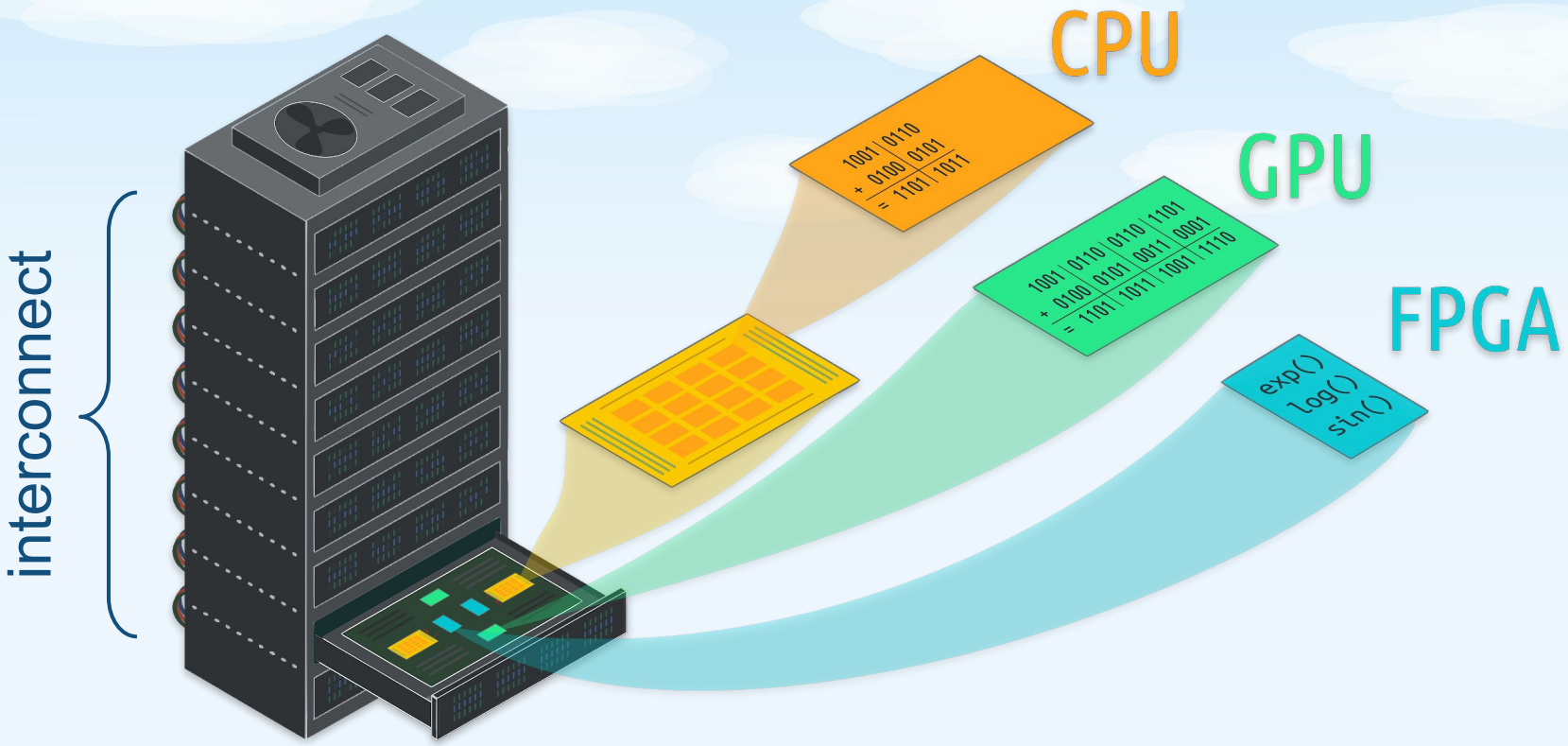
Modern high-performance architecture



Modern high-performance architecture



Modern high-performance architecture



Magritte's accelerator support

(At least) GPU acceleration for the main solver

	Host (CPU)	**Accelerator (GPU)**
Setup 1	AMD EPYC Rome	AMD Radeon Instinct MI50
Setup 2	Intel Skylake	Nvidia Tesla V100
Setup 3	Intel Skylake	Nvidia Tesla P100

Magritte

A **modern** software library for **3D radiative transfer**

RT solver

Magritte

A **modern** software library for **3D radiative transfer**

Magritte's mesher

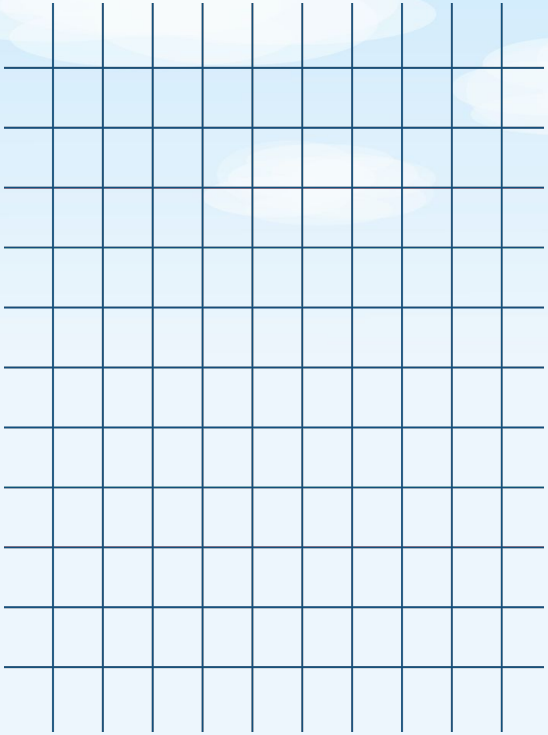
Questions:

*"How to **represent** the object on a computer?"*

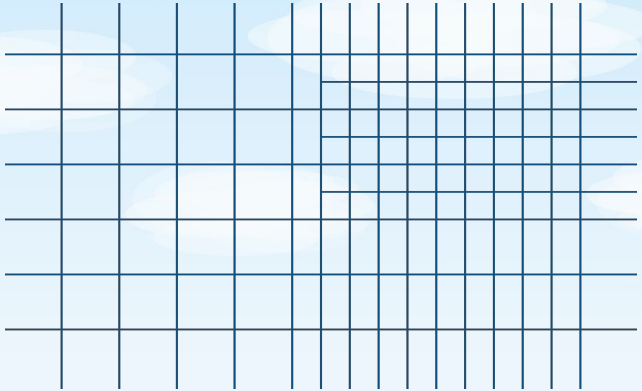
Note:

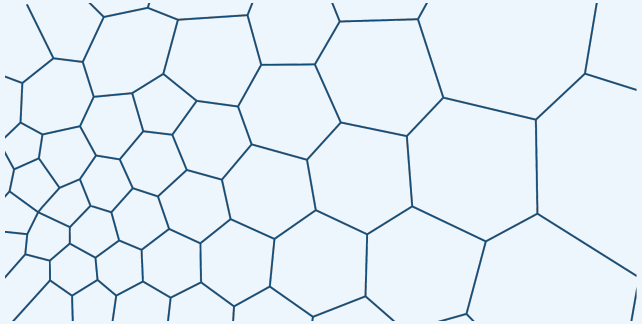
*"The representation is the source of **numerical errors**!"*

Magritte's mesher



structured





unstructured

SPH

Magritte's mesher

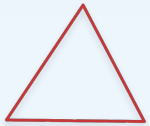
Magritte's **geometric data structure** only contains

- cell / point locations

- nearest neighbour lists

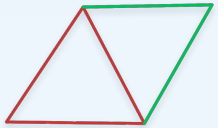
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



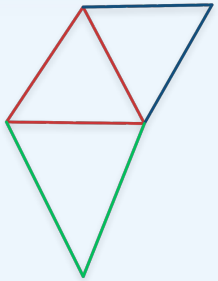
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



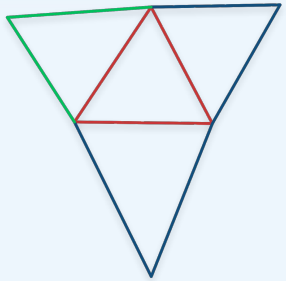
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



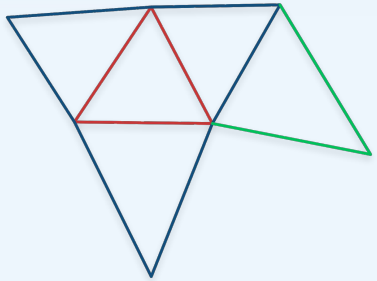
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



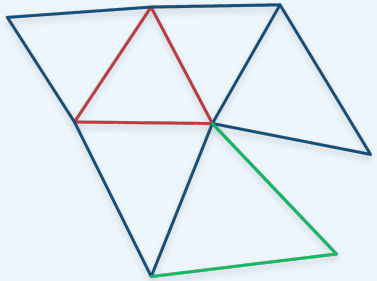
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



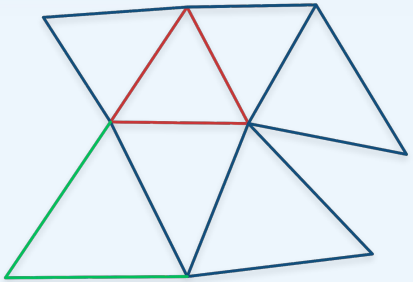
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



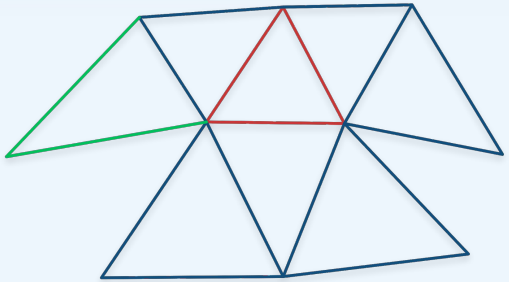
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



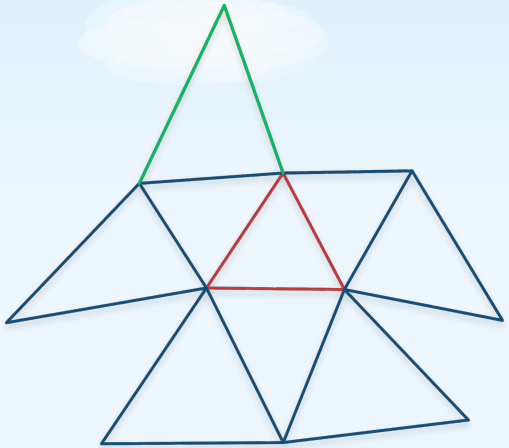
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



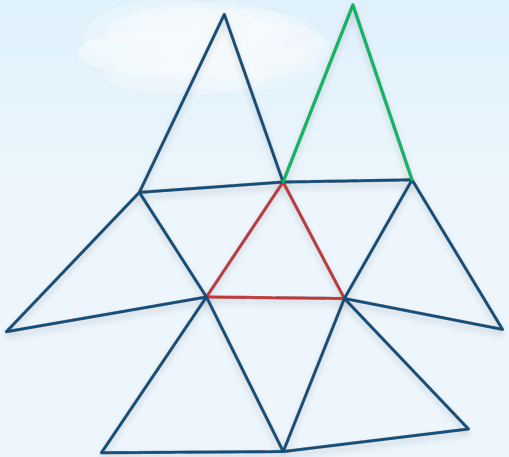
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



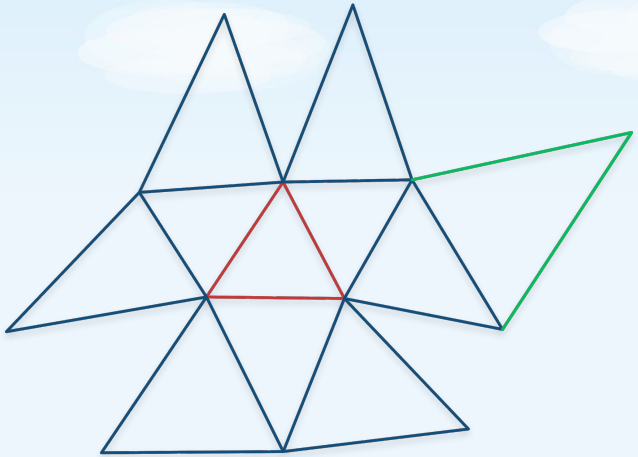
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



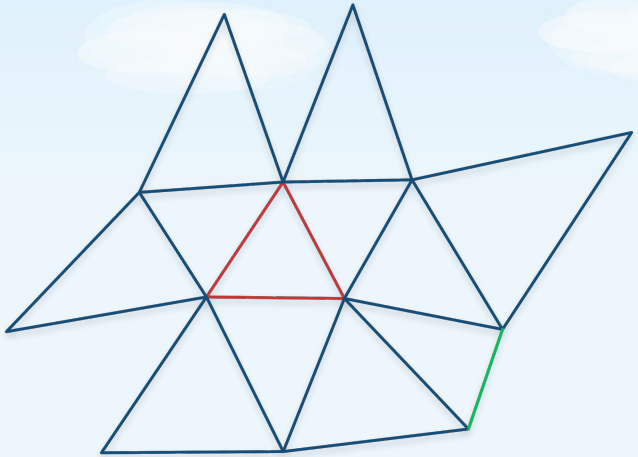
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



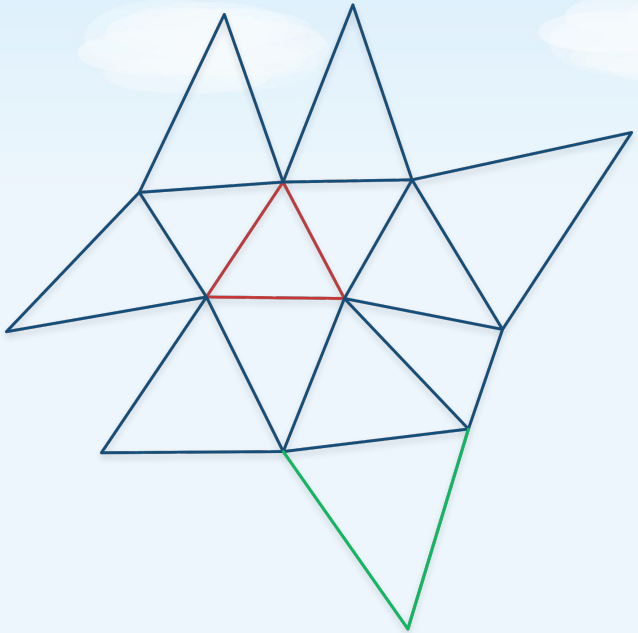
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



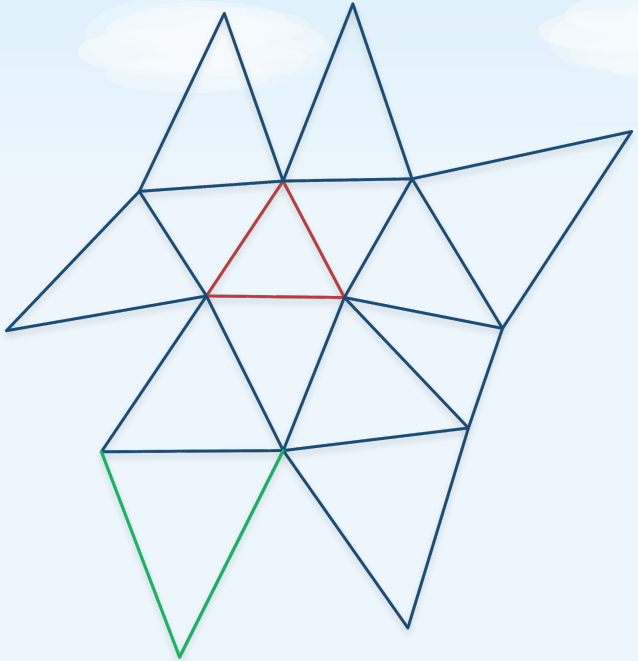
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



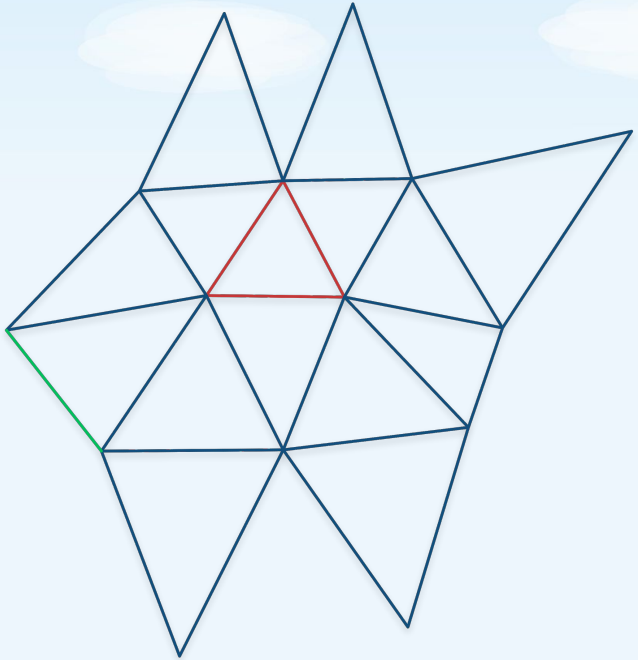
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



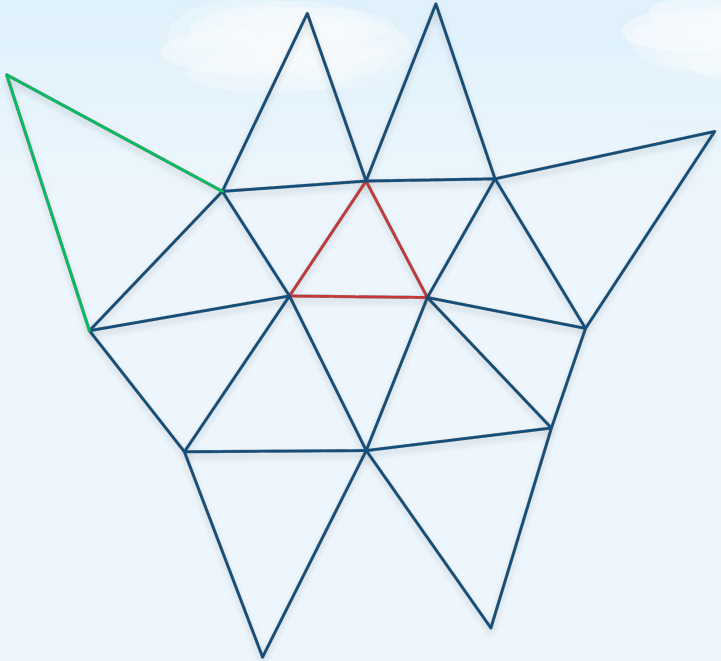
Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



Magritte's mesher

*"**Grow** the mesh from a **seed** by advancing the **front**"*



Magritte's mesher

How to **define the shape** of a new triangle?

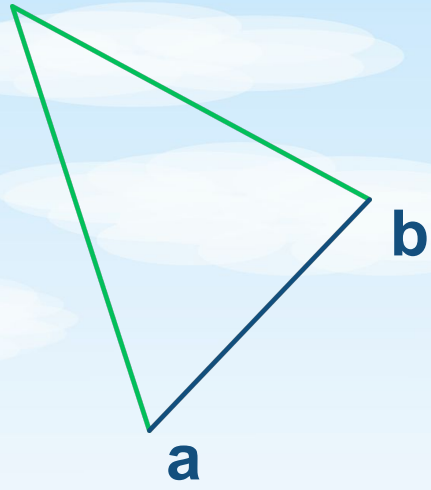
- *"Define the desired properties as a **heuristic**"*
- *"Determine the triangle by **optimising** the heuristic"*

Magritte's mesher

Example

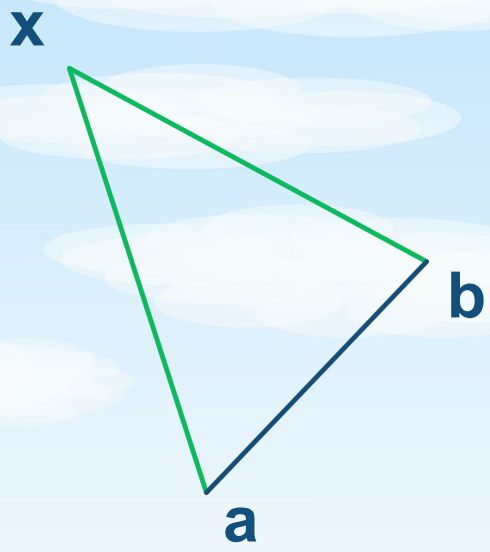
Magritte's mesher

Example

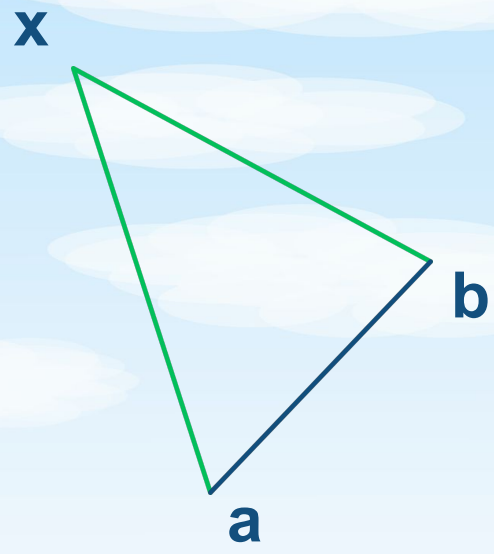


Magritte's mesher

Example



Magritte's mesher



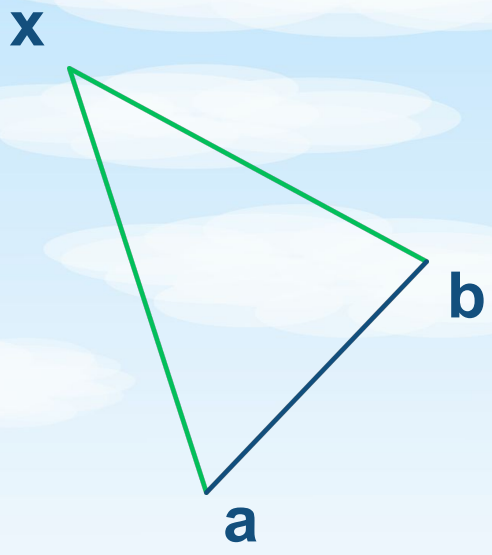
Example

Desired property edge length ≈ L

Heuristic $h(\mathbf{a},\mathbf{b},\mathbf{x}) = (|\mathbf{a}-\mathbf{x}| - L)^2 + (|\mathbf{b}-\mathbf{x}| - L)^2$

Find **x** by minimising $h(\mathbf{a},\mathbf{b},\mathbf{x})$ as function of **x**

Magritte's mesher



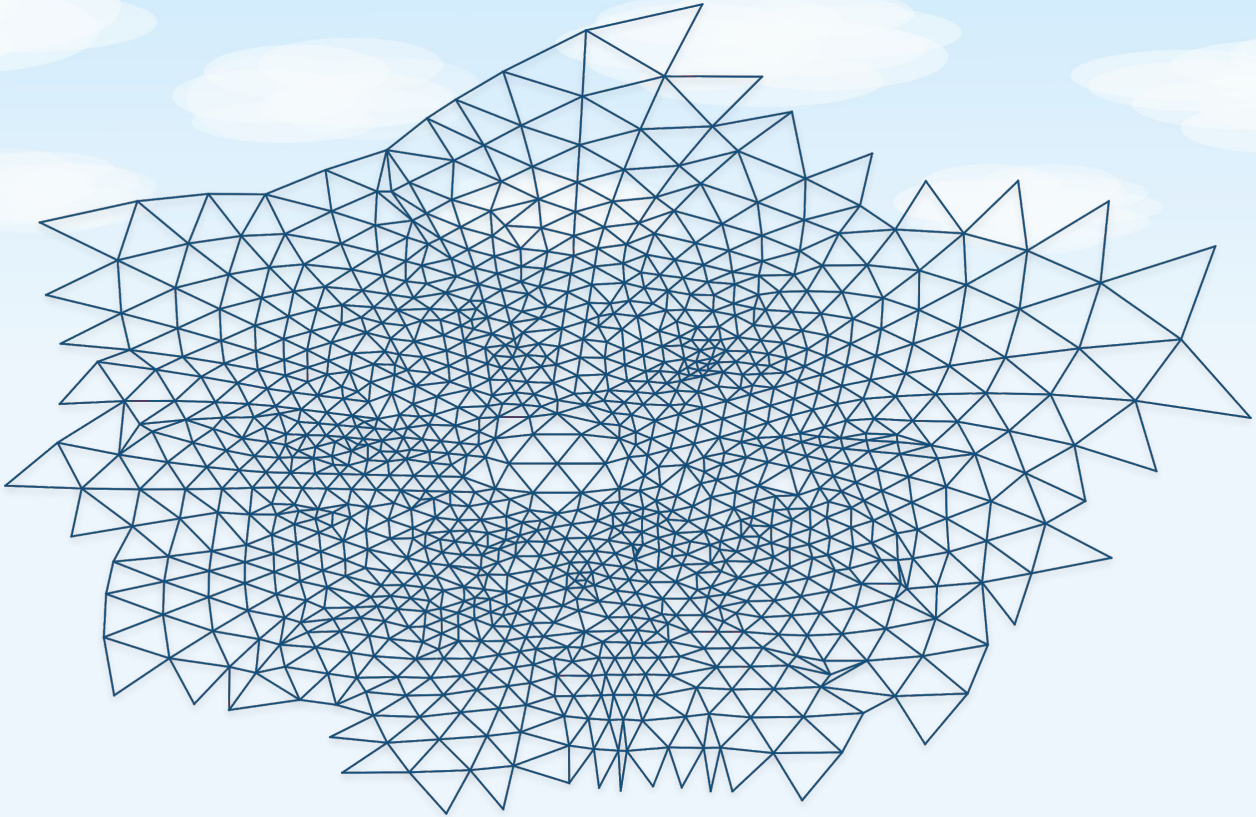
Example

Desired property edge length ≈ $L(\mathbf{x})$

Heuristic $h(\mathbf{a},\mathbf{b},\mathbf{x}) = (|\mathbf{a}-\mathbf{x}| - L(\mathbf{x}))^2 + (|\mathbf{b}-\mathbf{x}| - L(\mathbf{x}))^2$

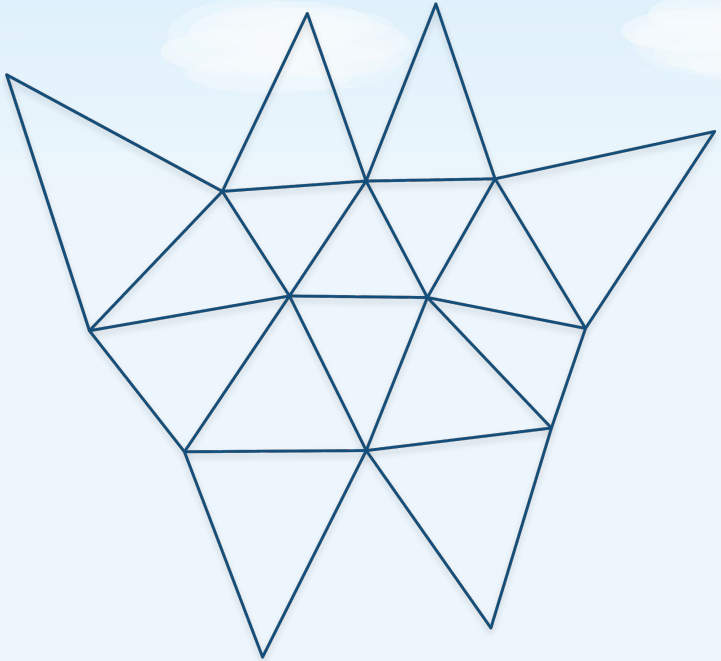
Find **x** by minimising $h(\mathbf{a},\mathbf{b},\mathbf{x})$ as function of **x**

Magritte's mesher



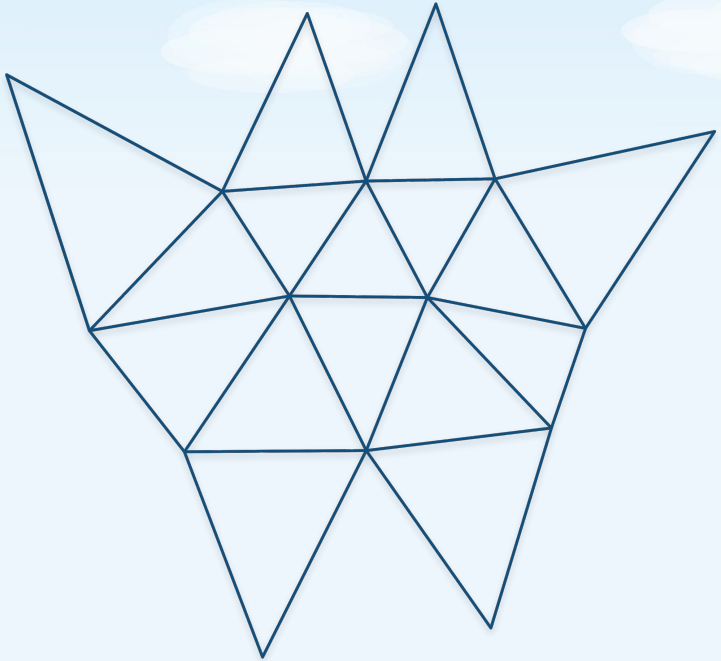
Magritte's mesher

*"How does this help in **constraining numerical errors**?"*



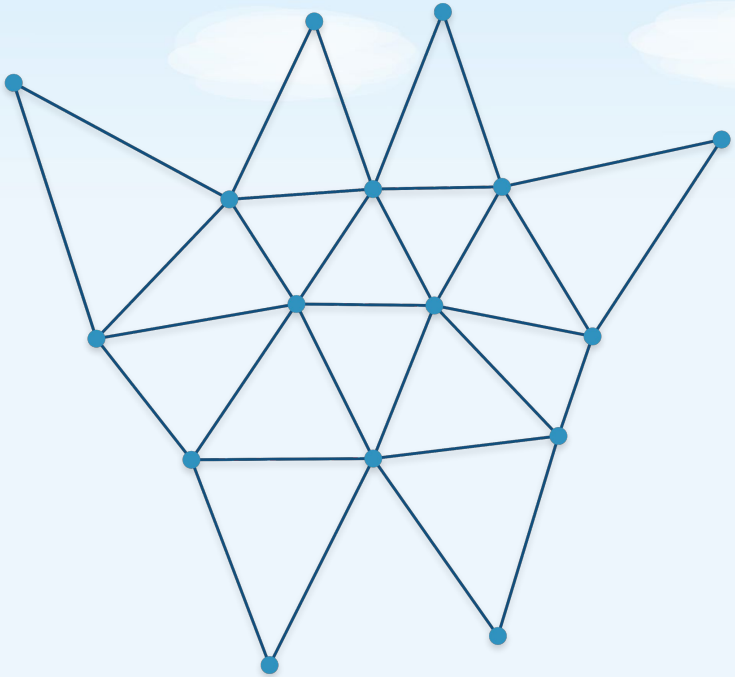
Magritte's mesher

"Triangulation determines point locations and neighbours"



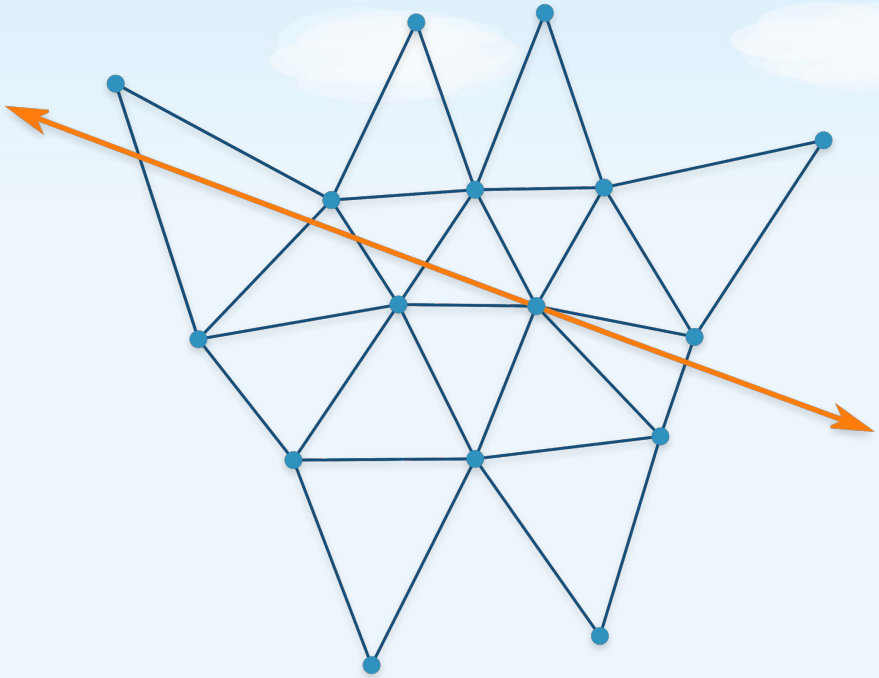
Magritte's mesher

"Triangulation determines point locations and neighbours"



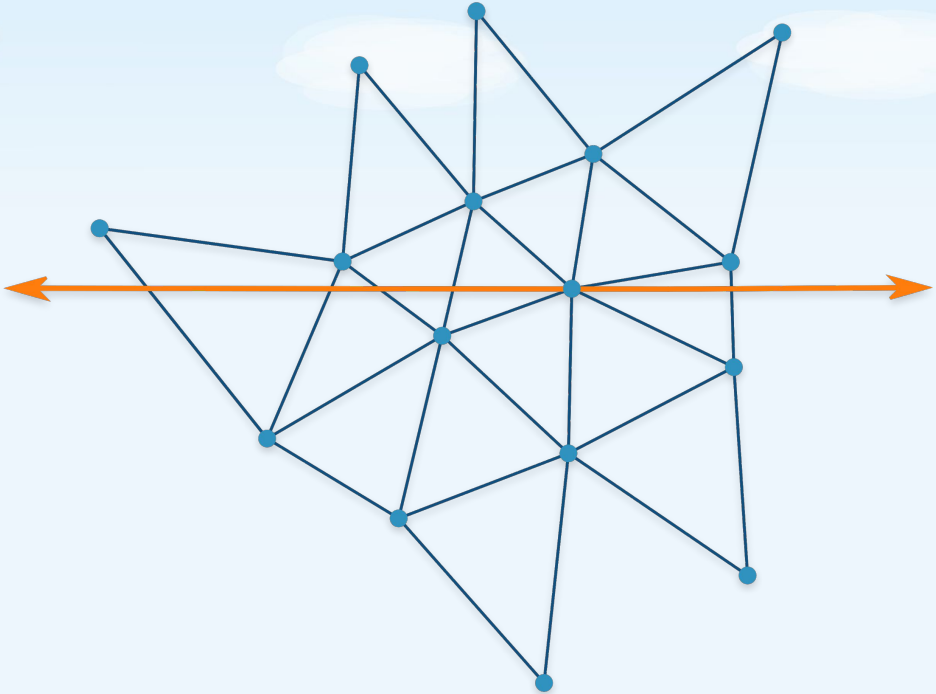
Magritte's mesher

*"Triangulation determines ray **step size ≤ edge length**"*



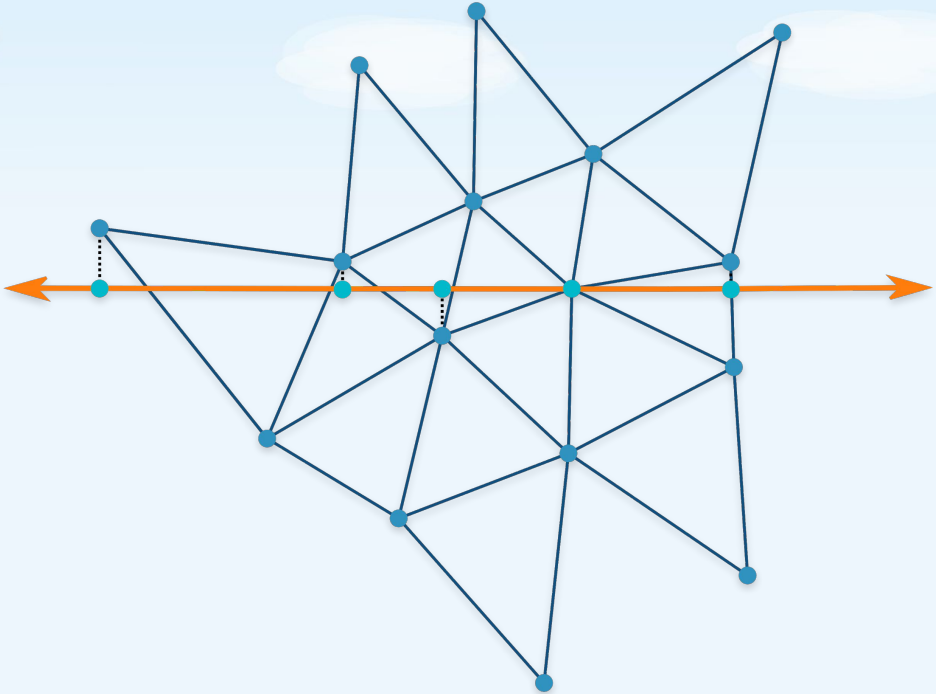
Magritte's mesher

*"Triangulation determines ray **step size ≤ edge length**"*



Magritte's mesher

*"Triangulation determines ray **step size ≤ edge length**"*

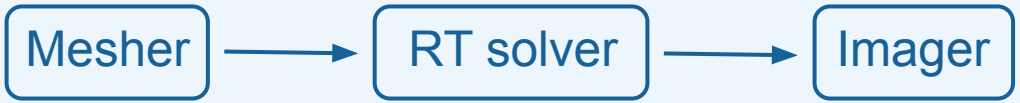


Magritte

A **modern** software library for **3D radiative transfer**

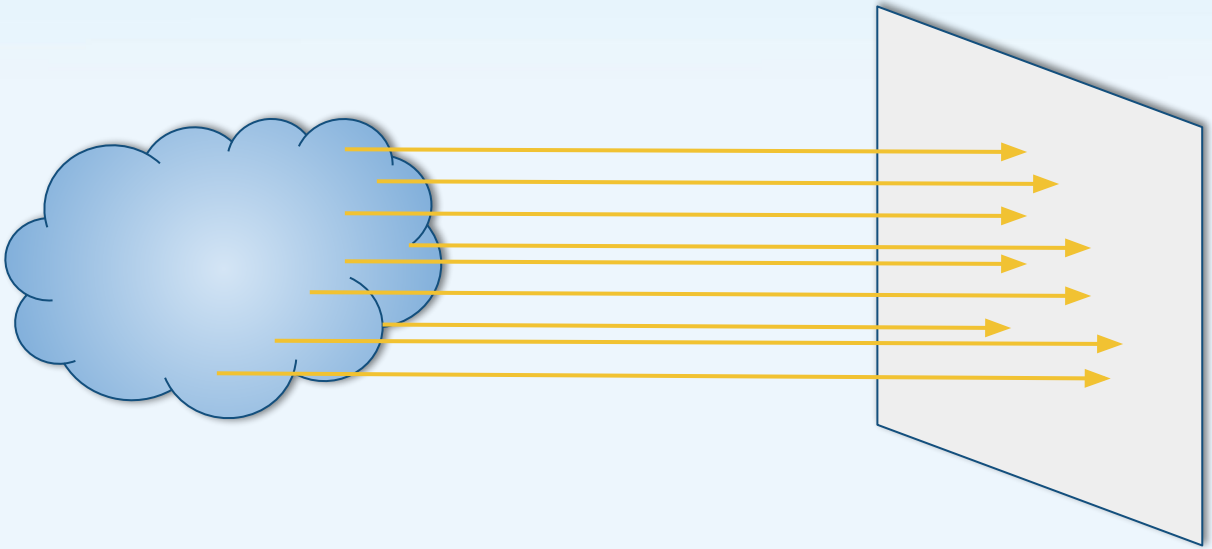
Magritte

A **modern** software library for **3D radiative transfer**

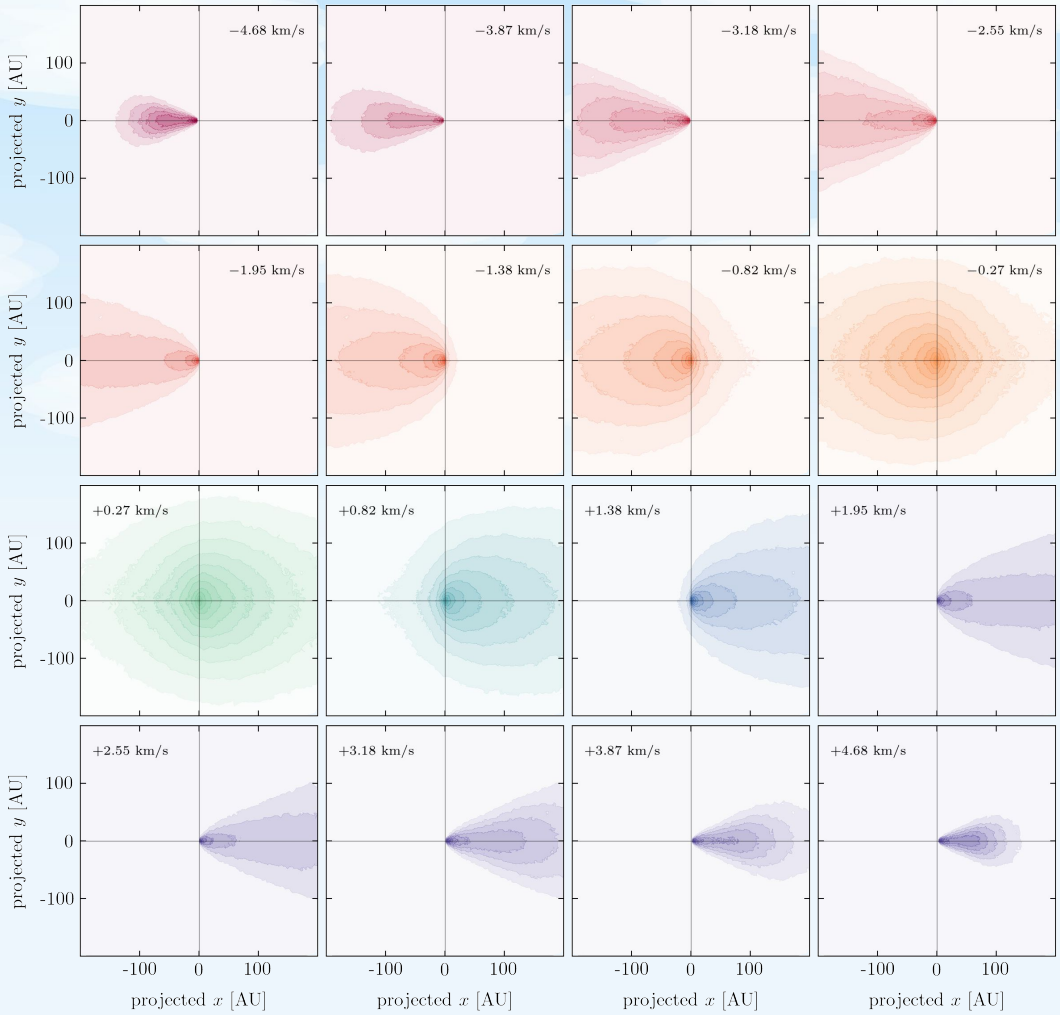


Magritte's imager

*"**Collect** all radiation that leaves the model in a certain direction and **project** it on a screen"*

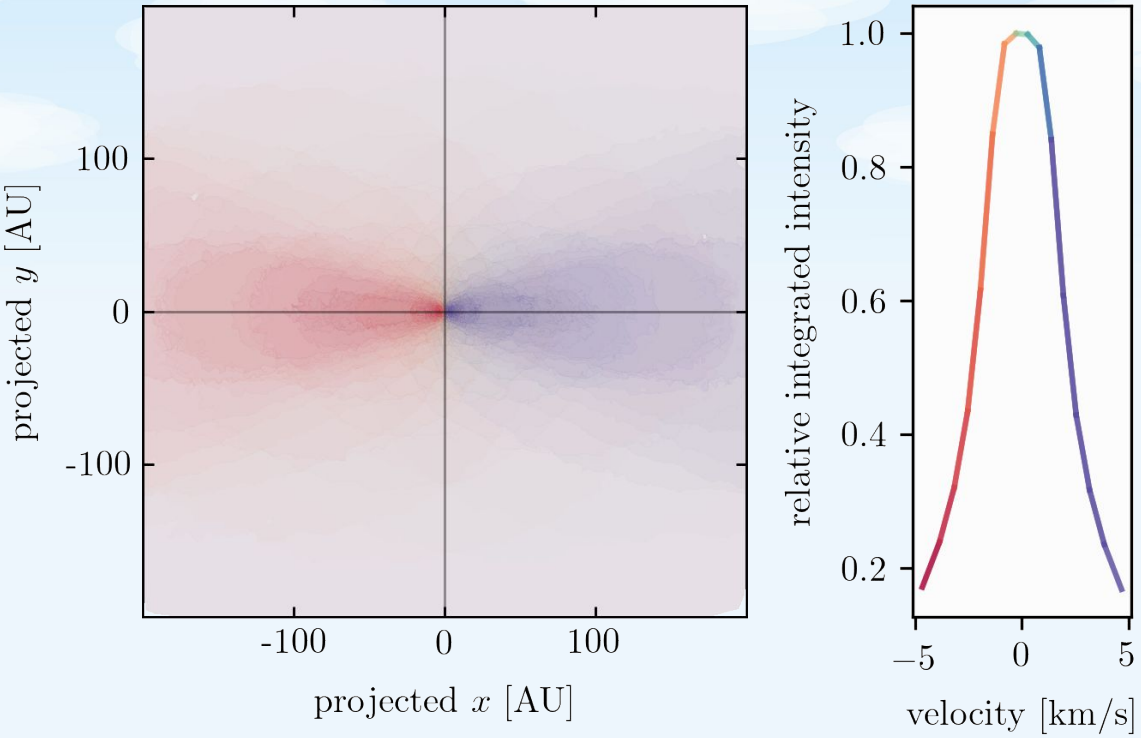


Magritte



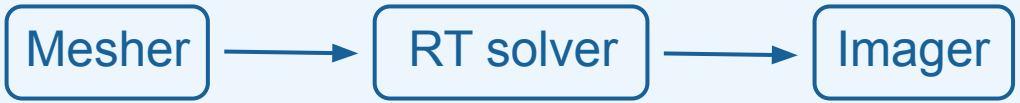
Channel maps of a Keplerian Disk (CO *J=1-0* line)

Magritte's imager



Magritte

A **modern** software library for **3D radiative transfer**



Magritte

A **modern** software library for **3D radiative transfer**

Magritte

A **modern** software library for 3D radiative transfer

Magritte

A **modern** software library for 3D radiative transfer

Magritte's status

Magritte's status

First paper submitted to MNRAS

Non-LTE atomic and molecular line modelling

- **Implementation** of line radiative transfer
- Semi-analytic **tests** and cross-code **benchmarks**
- **Application** to a Keplerian disk model

Magritte vs. Lime *(Brinch & Hogerheijde 2010)*

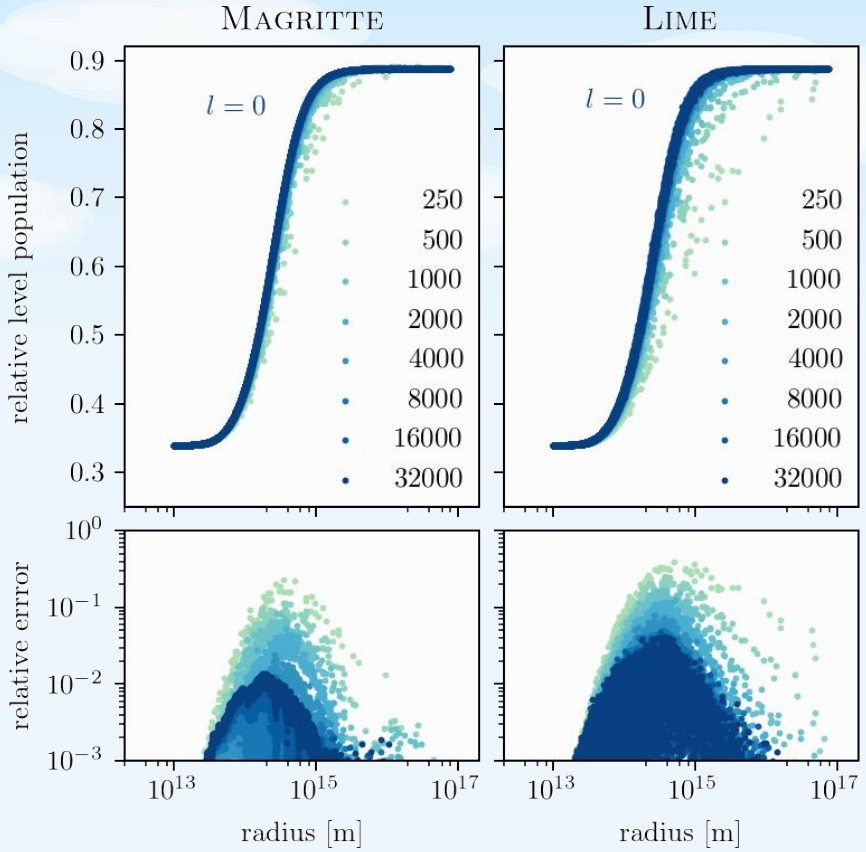
Benchmark 1a

(van Zadelhoff et al. 2002)

Magritte is

- More accurate
- More precise
- (1.6x faster)

than Lime



Magritte vs. Lime *(Brinch & Hogerheijde 2010)*

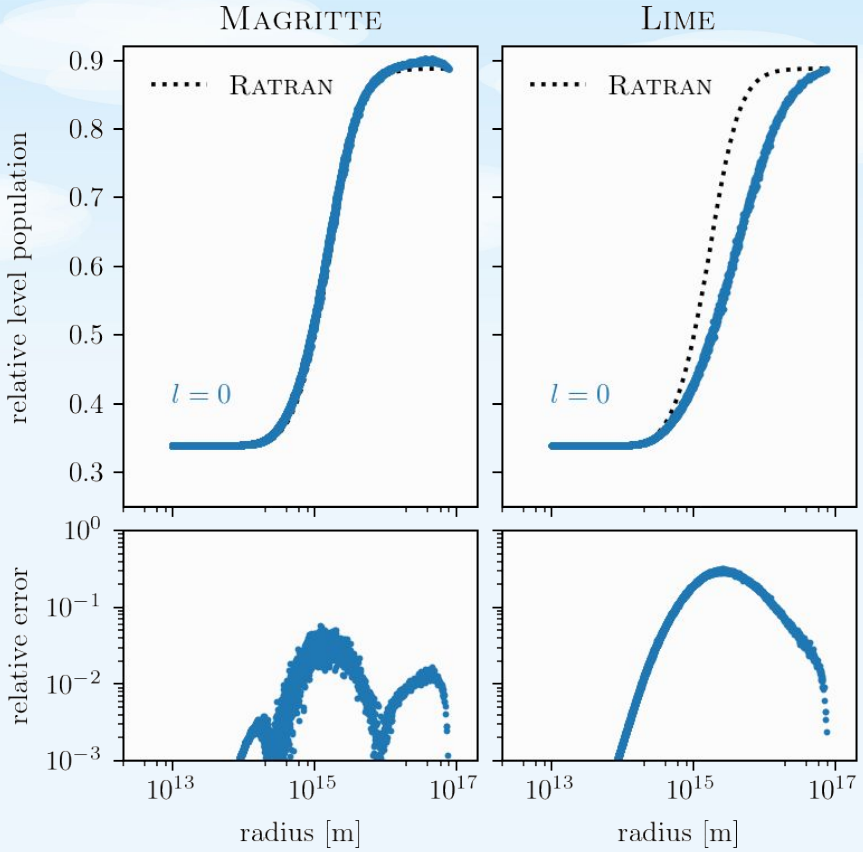
Benchmark 1b

(van Zadelhoff et al. 2002)

Magritte is

- More accurate
- More precise
- (1.6x faster)

than Lime



Magritte's status

First paper submitted to MNRAS

Non-LTE atomic and molecular line modelling

Second paper in prep.

Design strategy and performance analysis

Magritte

Magritte

Magritte

Thanks!

github.com/Magritte-code

@FredDeCeuster

@FredDeCeuster