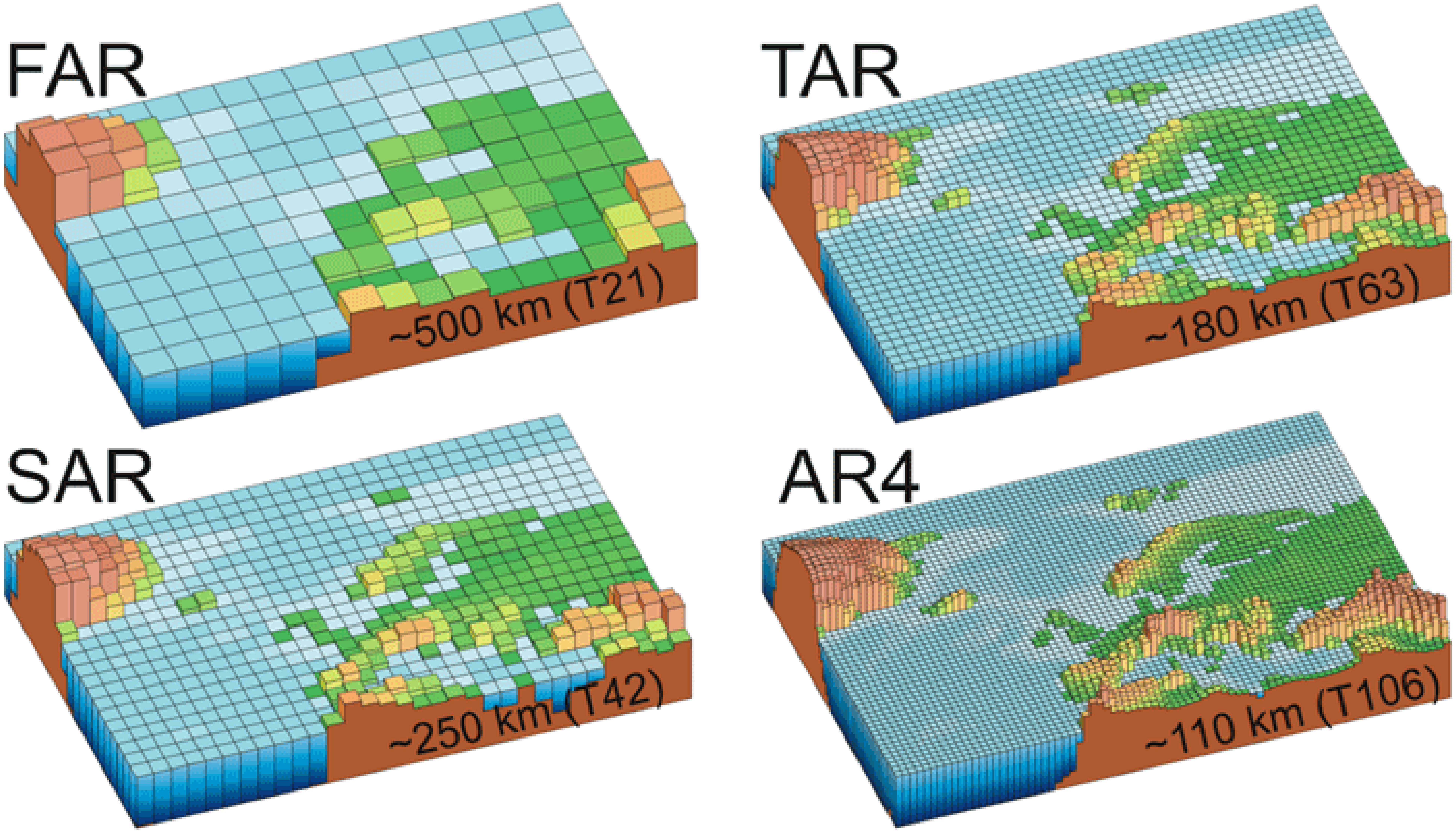
Climate change and sustainability
How Research Software Engineering can help

Paul Richmond
Engineering Lead, ICCS, University of Cambridge

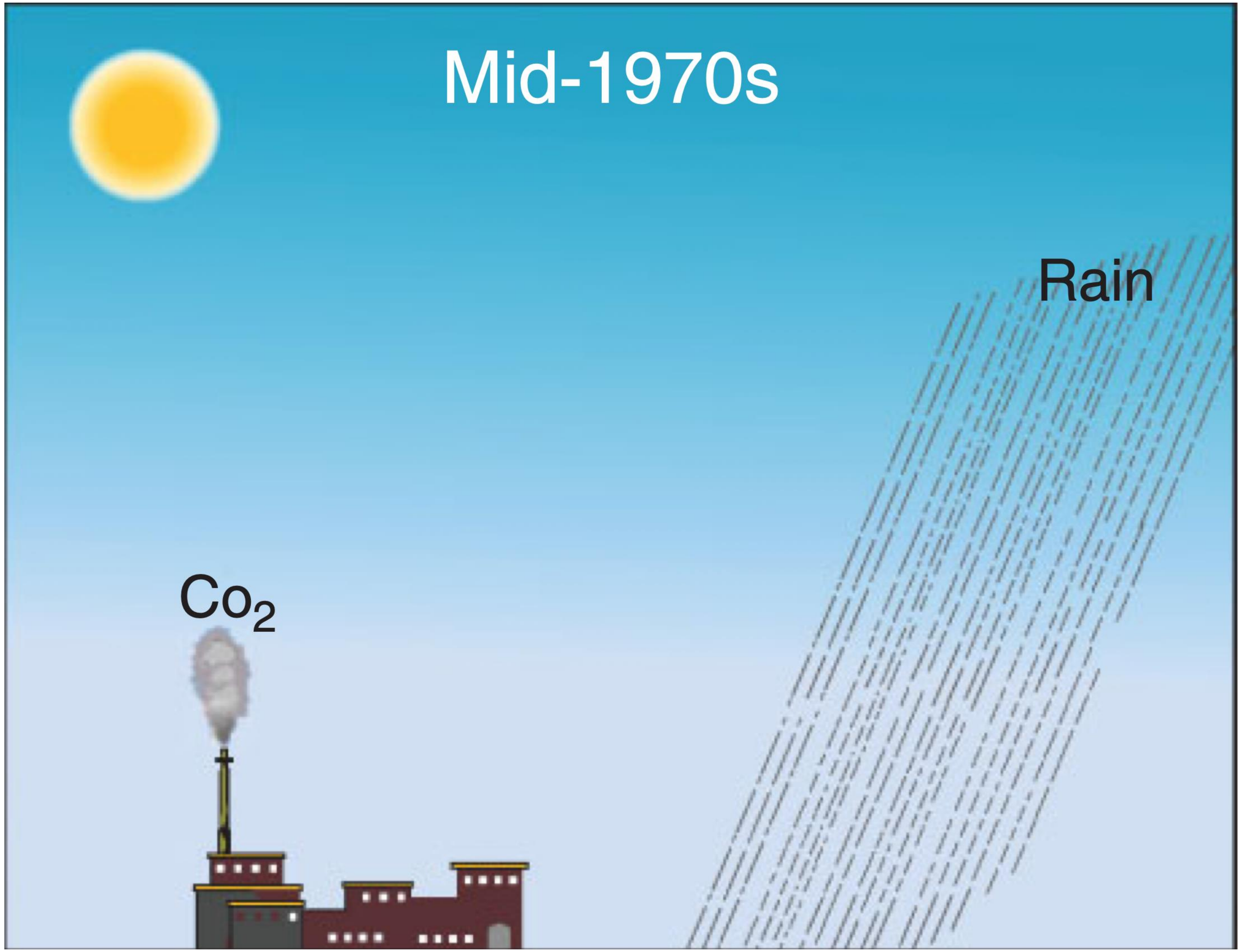
1850-2021 (Ed Hawkins “Warming stripes”)

Increasing resolution

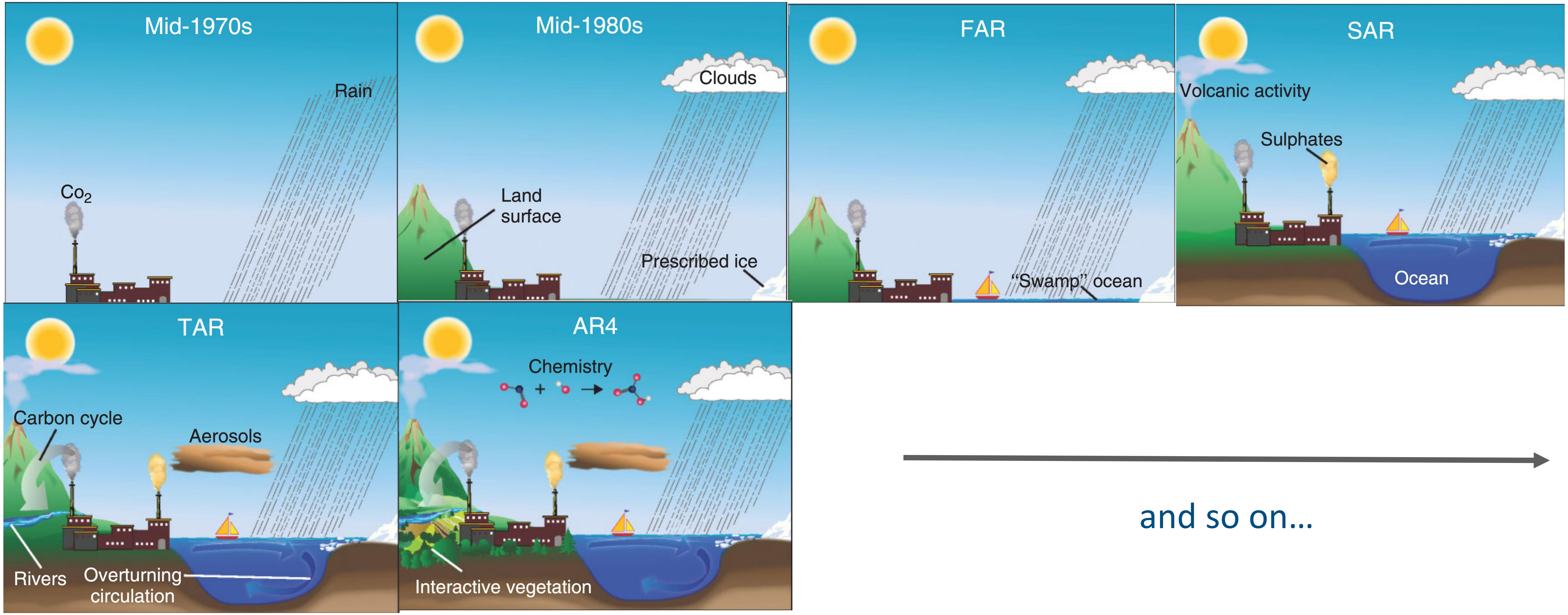


graphics from 4th IPCC report (2007)

Increasing process complexity

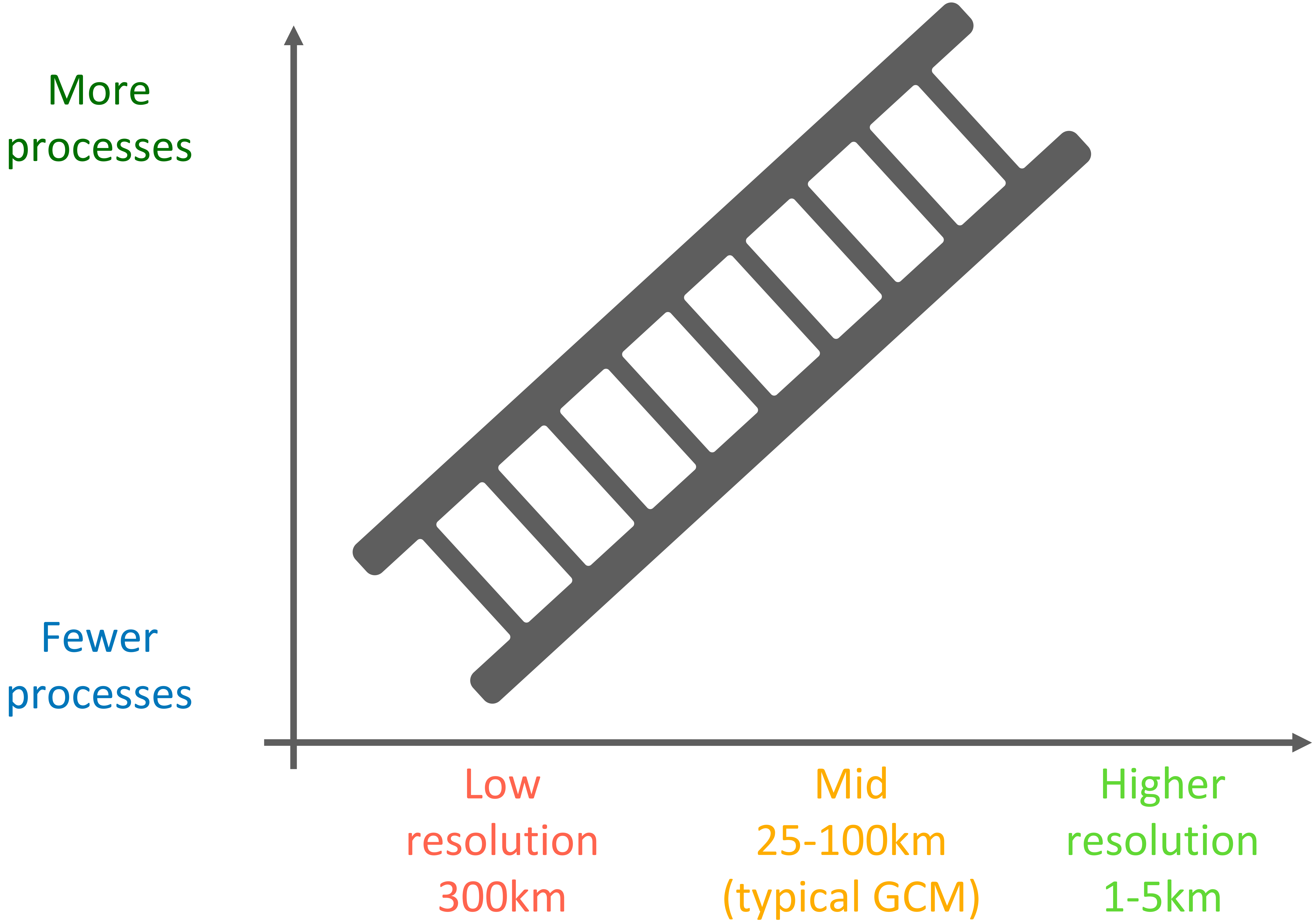


Increasing process complexity

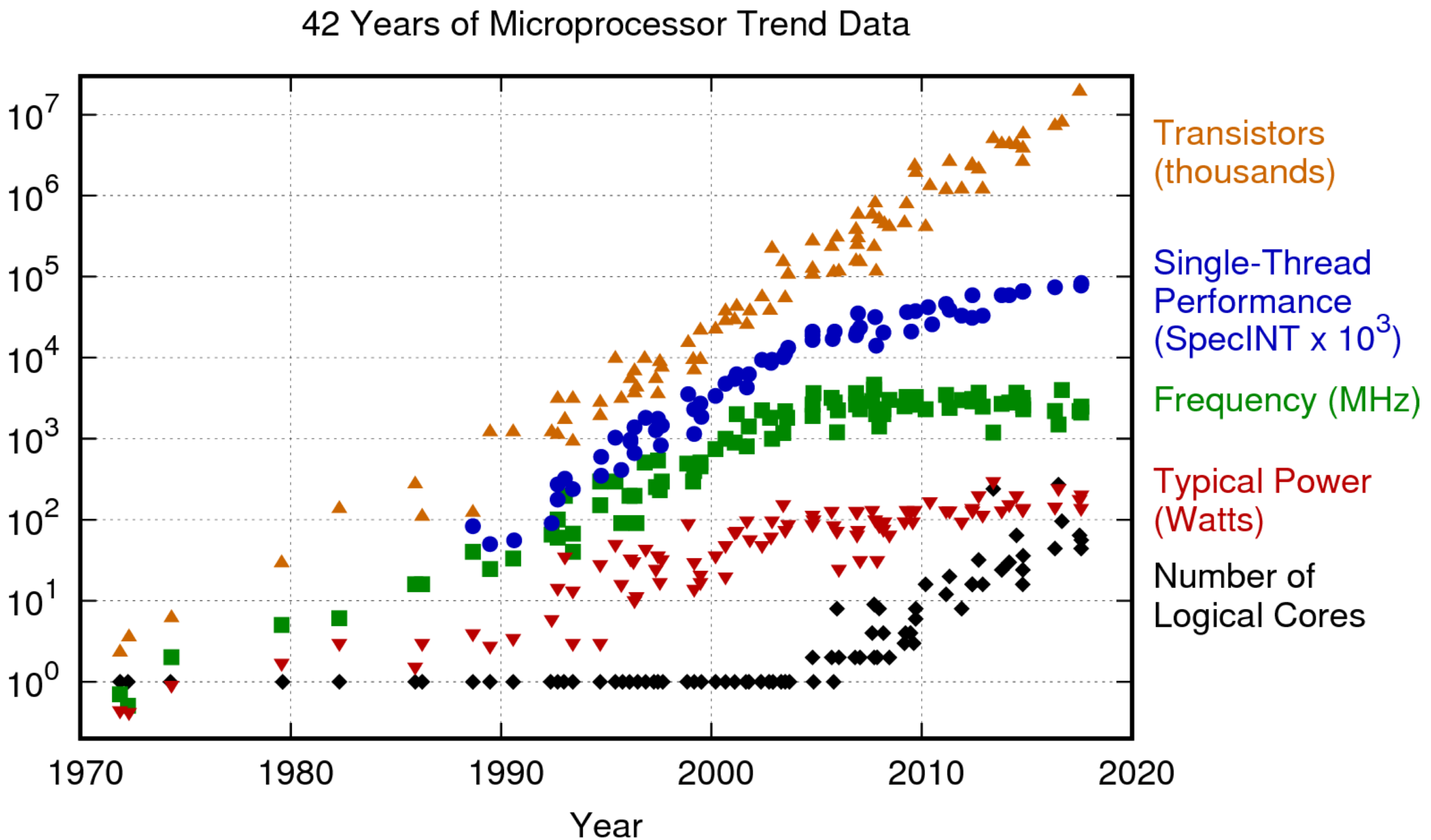


and so on…

Better prediction: “climbing the ladder” (Charney)

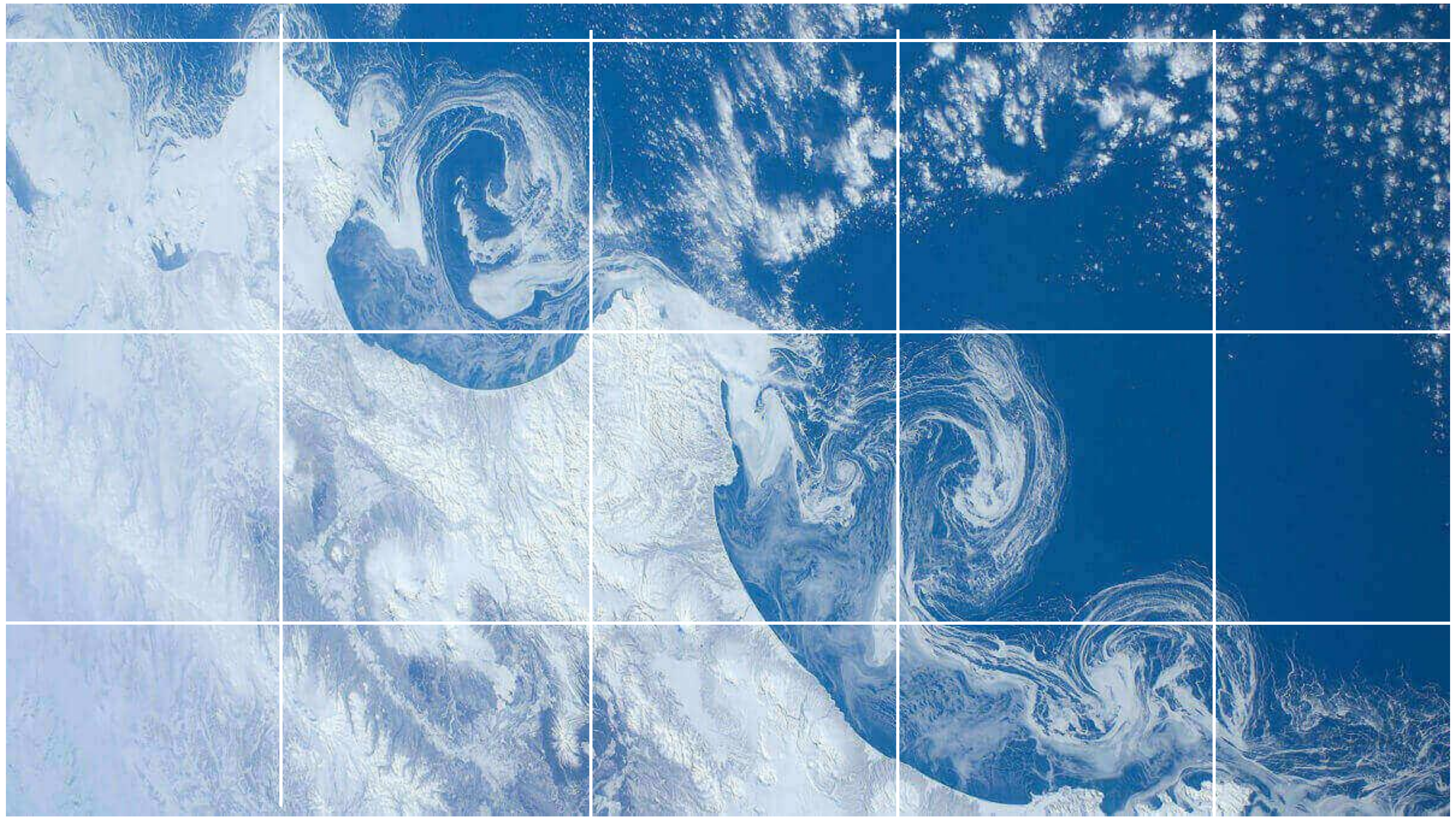


Scaling computational performance



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2017 by K. Rupp

Approximating sub grid processes



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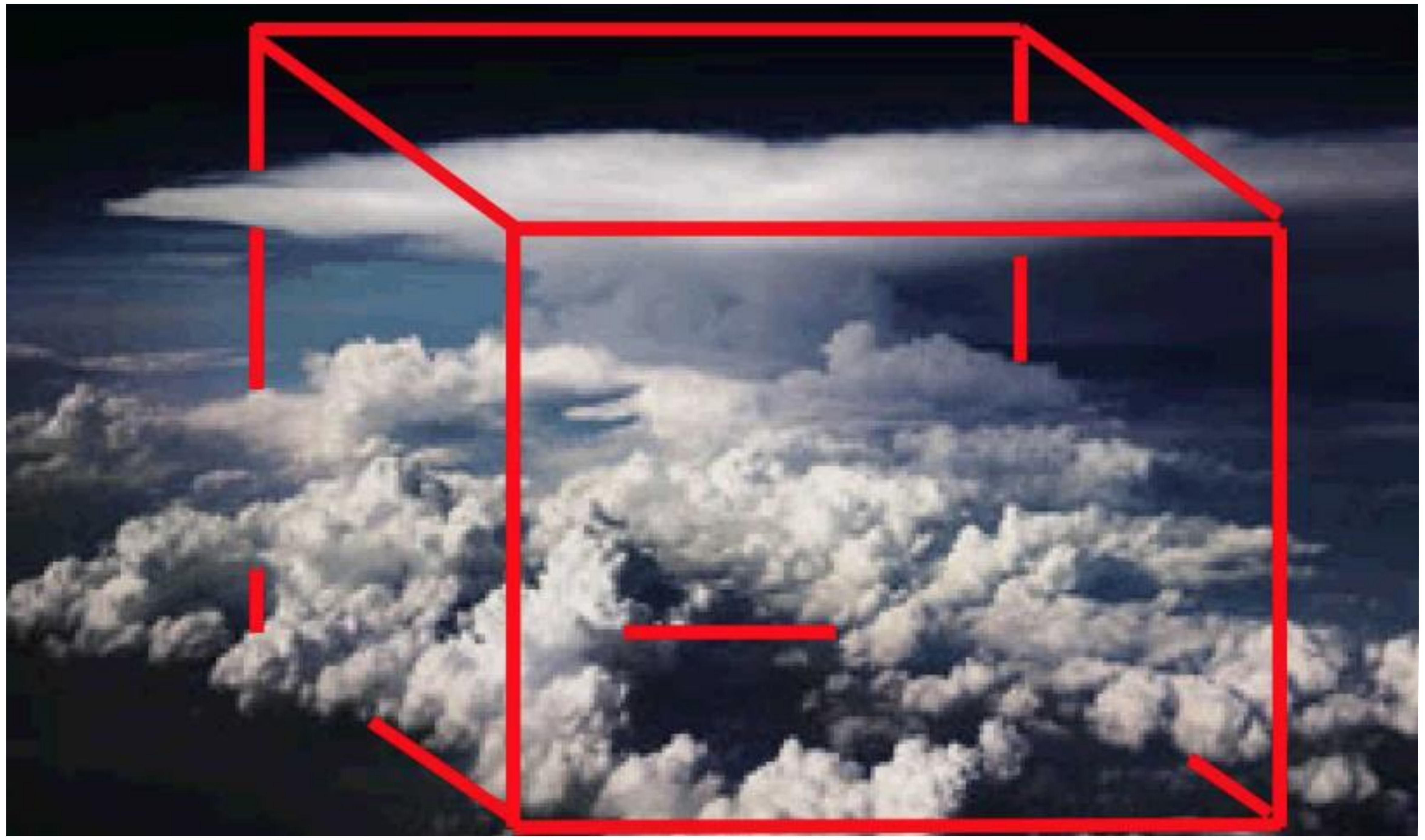
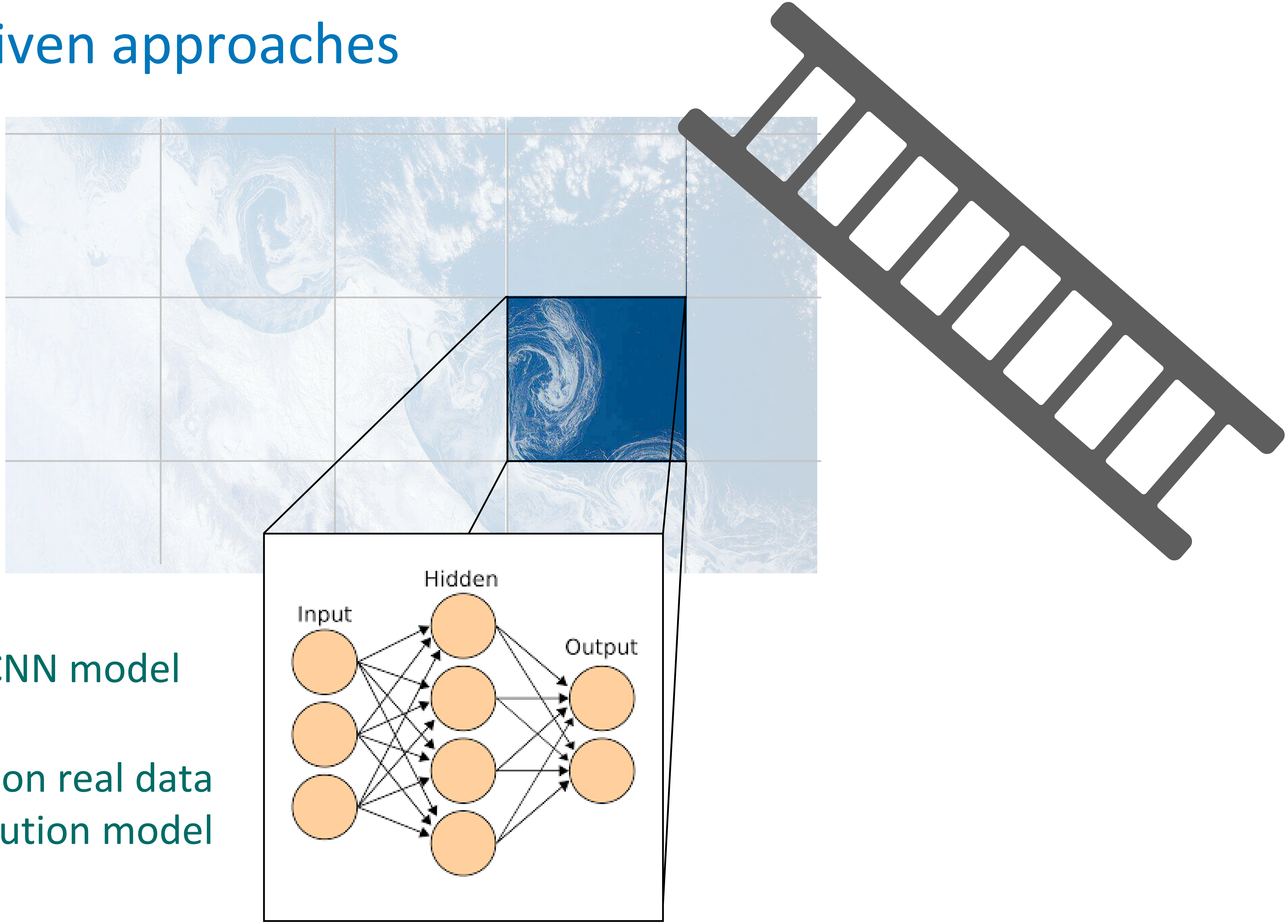


Hillman et al. 2020

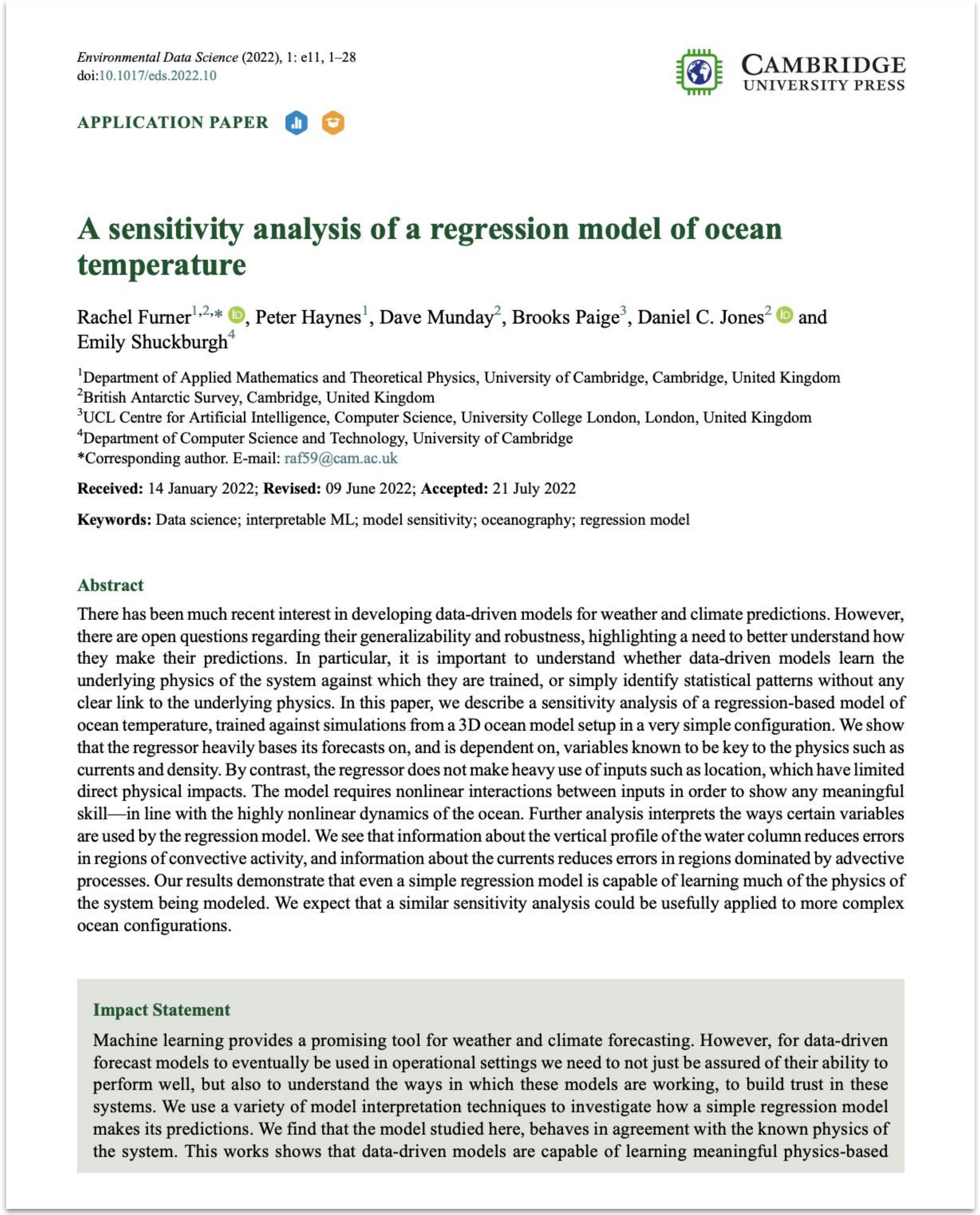
Data-driven approaches



CNN model

Train on real data
or high-resolution model

Ensuring reproducible research



Environmental Data Science (2022), 1: e11, 1–28
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APPLICATION PAPER

A sensitivity analysis of a regression model of ocean temperature

Rachel Furner[1,2,*], Peter Haynes[1], Dave Munday[2], Brooks Paige[3], Daniel C. Jones[2] and Emily Shuckburgh[4]

[1]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, United Kingdom
[2]British Antarctic Survey, Cambridge, United Kingdom
[3]UCL Centre for Artificial Intelligence, Computer Science, University College London, London, United Kingdom
[4]Department of Computer Science and Technology, University of Cambridge
*Corresponding author. E-mail: raf59@cam.ac.uk

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Keywords: Data science; interpretable ML; model sensitivity; oceanography; regression model

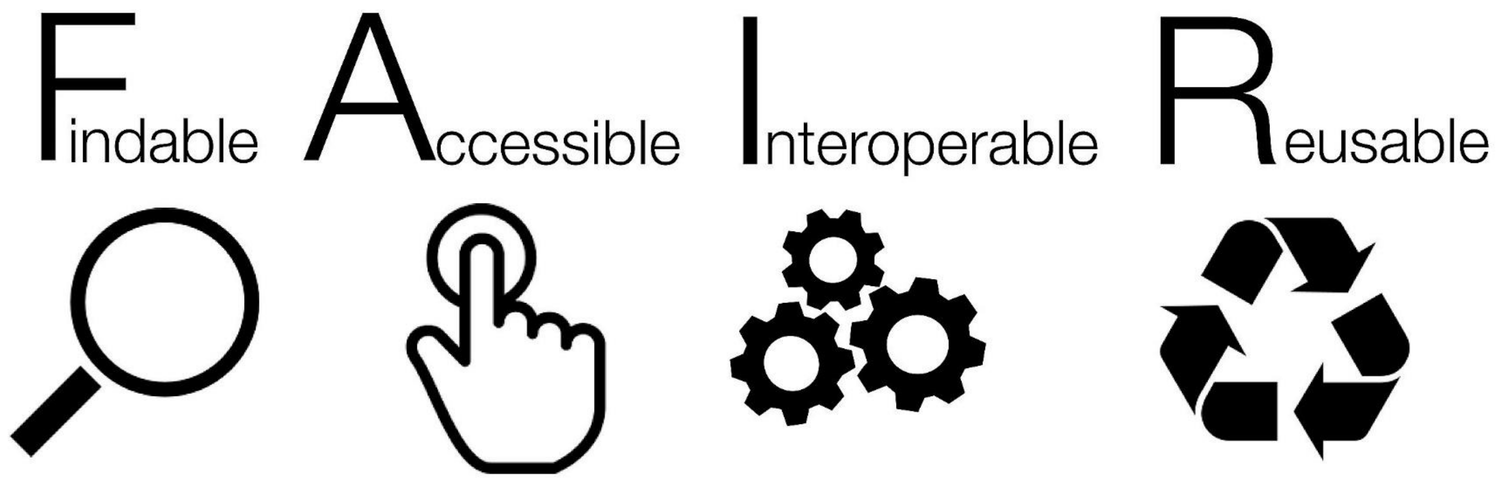
Abstract

There has been much recent interest in developing data-driven models for weather and climate predictions. However, there are open questions regarding their generalizability and robustness, highlighting a need to better understand how they make their predictions. In particular, it is important to understand whether data-driven models learn the underlying physics of the system against which they are trained, or simply identify statistical patterns without any clear link to the underlying physics. In this paper, we describe a sensitivity analysis of a regression-based model of ocean temperature, trained against simulations from a 3D ocean model setup in a very simple configuration. We show that the regressor heavily bases its forecasts on, and is dependent on, variables known to be key to the physics such as currents and density. By contrast, the regressor does not make heavy use of inputs such as location, which have limited direct physical impacts. The model requires nonlinear interactions between inputs in order to show any meaningful skill—in line with the highly nonlinear dynamics of the ocean. Further analysis interprets the ways certain variables are used by the regression model. We see that information about the vertical profile of the water column reduces errors in regions of convective activity, and information about the currents reduces errors in regions dominated by advective processes. Our results demonstrate that even a simple regression model is capable of learning much of the physics of the system being modeled. We expect that a similar sensitivity analysis could be usefully applied to more complex ocean configurations.

Impact Statement

Machine learning provides a promising tool for weather and climate forecasting. However, for data-driven forecast models to eventually be used in operational settings we need to not just be assured of their ability to perform well, but also to understand the ways in which these models are working, to build trust in these systems. We use a variety of model interpretation techniques to investigate how a simple regression model makes its predictions. We find that the model studied here, behaves in agreement with the known physics of the system. This works shows that data-driven models are capable of learning meaningful physics-based

```
module simulation_mod
  use helpers_mod
  implicit none

  contains

  subroutine compute_tentative_velocity(u, v, f, g, flag, del_t)
    real u(0:imax+1, 0:jmax+1), v(0:imax+1, 0:jmax+1), f(0:imax+1, 0:jmax+1),  &
         g(0:imax+1, 0:jmax+1)
    integer flag(0:imax+1, 0:jmax+1)
    real, intent(in) :: del_t

    integer i, j
    real du2dx, duvdy, duvdx, dv2dy, laplu, laplv

    do i = 1, (imax-1)
      do j = 1, jmax
        ! only if both adjacent cells are fluid cells */
        if (toLogical(iand(flag(i,j), C_F)) .and.                              &
            toLogical(iand(flag(i+1,j), C_F))) then

          du2dx = ((u(i,j)+u(i+1,j))*(u(i,j)+u(i+1,j))+                        &
                  gamma*abs(u(i,j)+u(i+1,j))*(u(i,j)-u(i+1,j))-                &
                  (u(i-1,j)+u(i,j))*(u(i-1,j)+u(i,j))-                         &
                  gamma*abs(u(i-1,j)+u(i,j))*(u(i-1,j)-u(i,j)))                &
                  /(4.0*delx)
          duvdy = ((v(i,j)+v(i+1,j))*(u(i,j)+u(i,j+1))+                        &
                  gamma*abs(v(i,j)+v(i+1,j))*(u(i,j)-u(i,j+1))-                &
                  (v(i,j-1)+v(i+1,j-1))*(u(i,j-1)+u(i,j))-                     &
                  gamma*abs(v(i,j-1)+v(i+1,j-1))*(u(i,j-1)-u(i,j)))            &
                      /(4.0*dely)
          laplu = (u(i+1,j)-2.0*u(i,j)+u(i-1,j))/delx/delx+                    &
                  (u(i,j+1)-2.0*u(i,j)+u(i,j-1))/dely/dely

          f(i,j) = u(i,j) + del_t*(laplu/Re-du2dx-duvdy)
        else
          f(i,j) = u(i,j)
        end if
      end do
    end do
```



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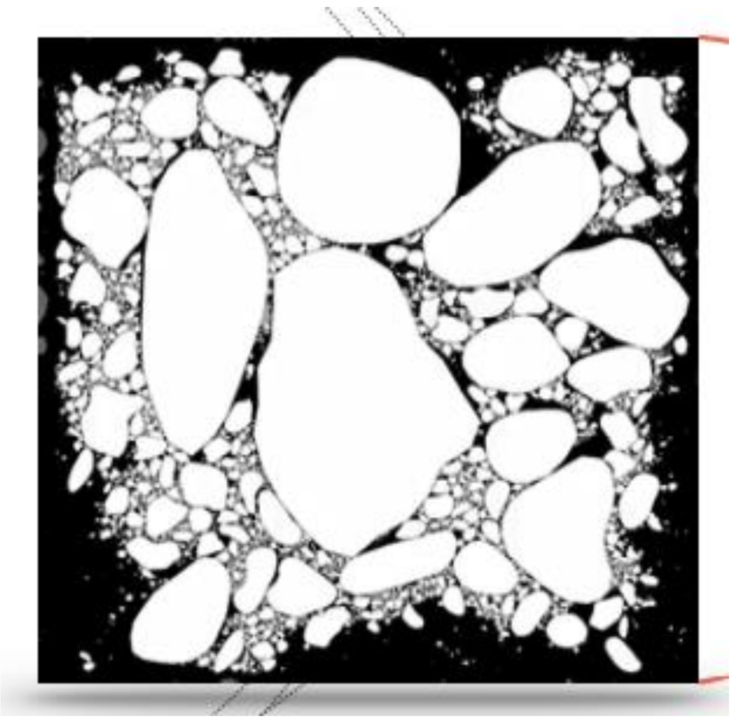
Virtual Institute for Scientific Software

VISS supports the launch of a network of scientific software engineering centers at several research universities that are working to accelerate the pace of scientific discovery.

Virtual Earth System Research Institute (VESRI)

VESRI aims to improve the accuracy and credibility of major climate models by addressing some of the hardest problems that challenge them.

DataWave



SASIP

LEMONTREE

M^{2}LInES

Emily Shuckburgh

Cambridge Zero
+ CST

Colm Caulfield

Department of Applied Maths and Theoretical Physics

Chris Edsall

University Information Services

Dominic Orchard

Department of Computer Science & Technology

Marla Fuchs

DAMTP

UNIVERSITY OF CAMBRIDGE

Institute of Computing for Climate Science

Research Software Engineers

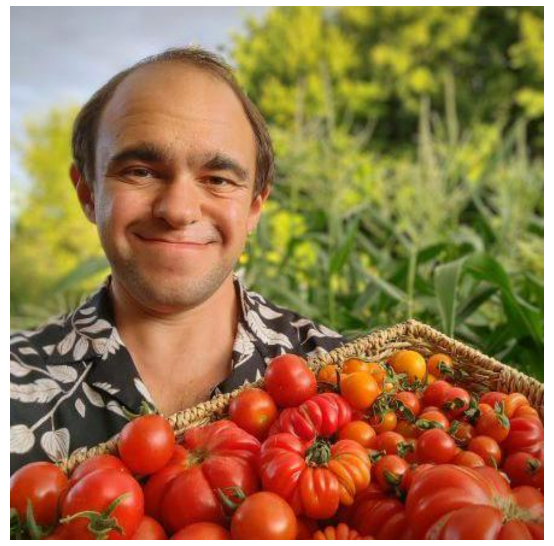
Kacper Kornet

Simon Clifford

Ben Orchard

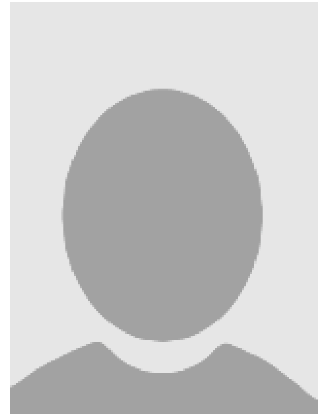
Matt Archer

Jack Atkinson



Alexander Smith

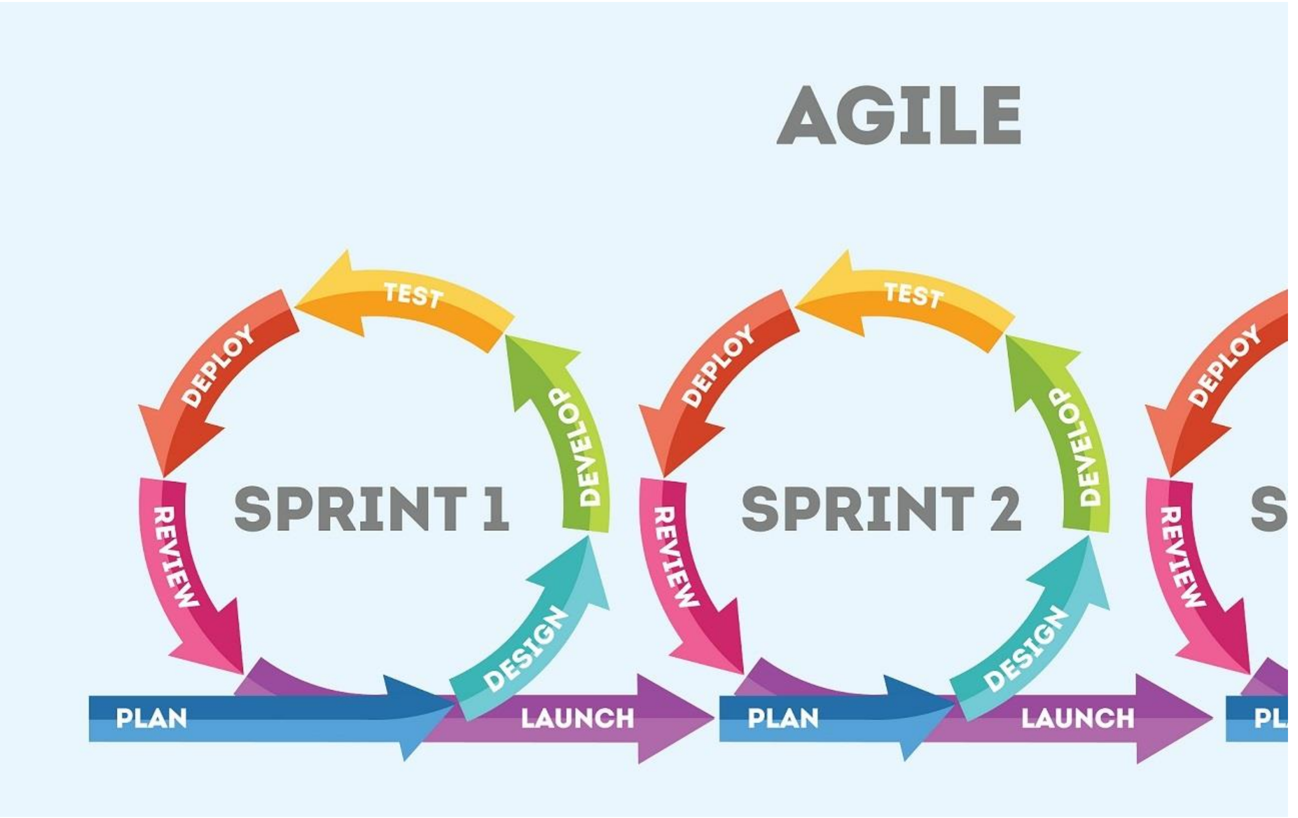
Paul Richmond



More on the way…

Software engineering tools & techniques

Processes



Version control & public curators

GitHub

GitLab

Build systems & containers

CMake

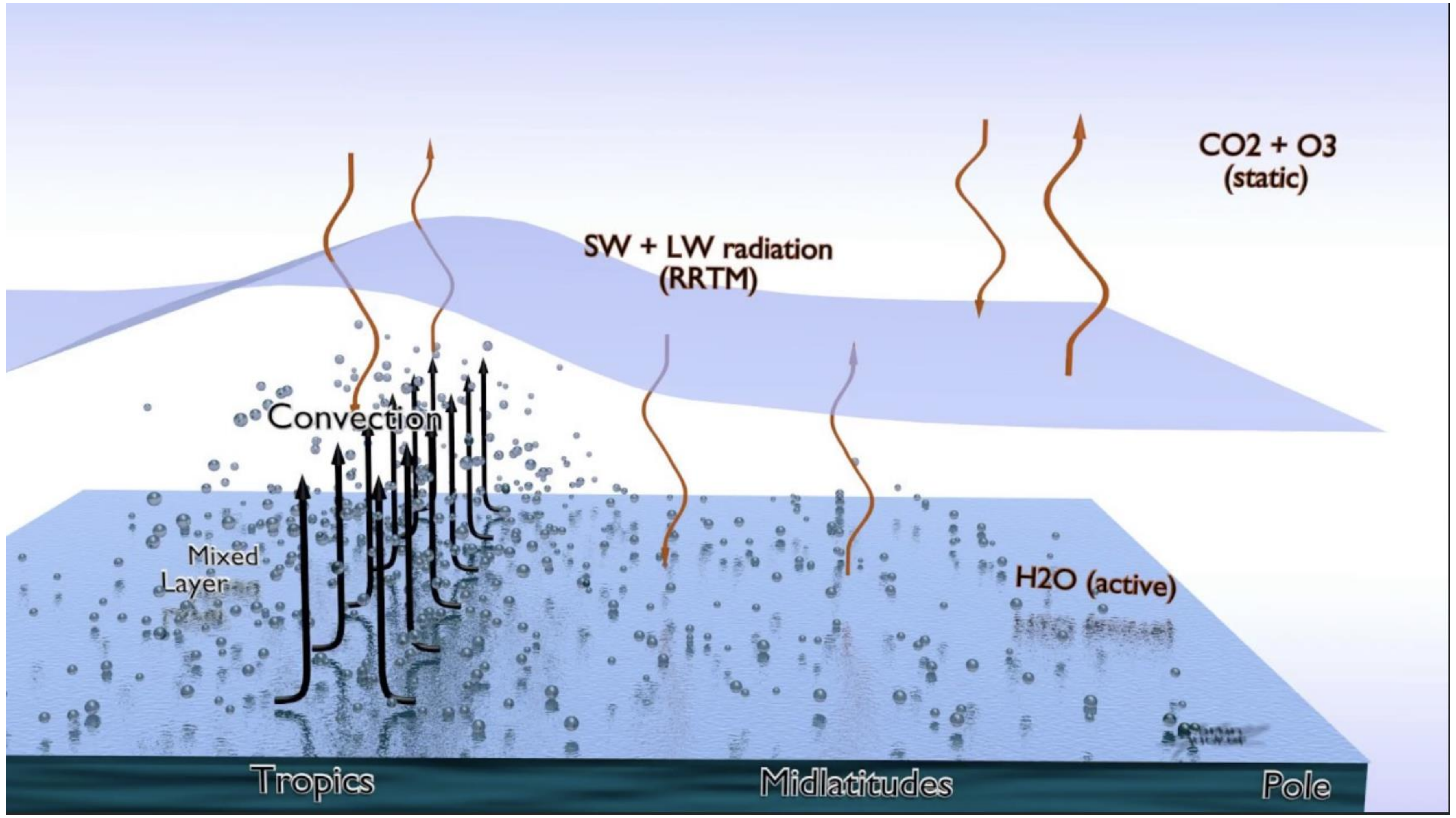
docker

Debugging

Profiling

Testing and verification

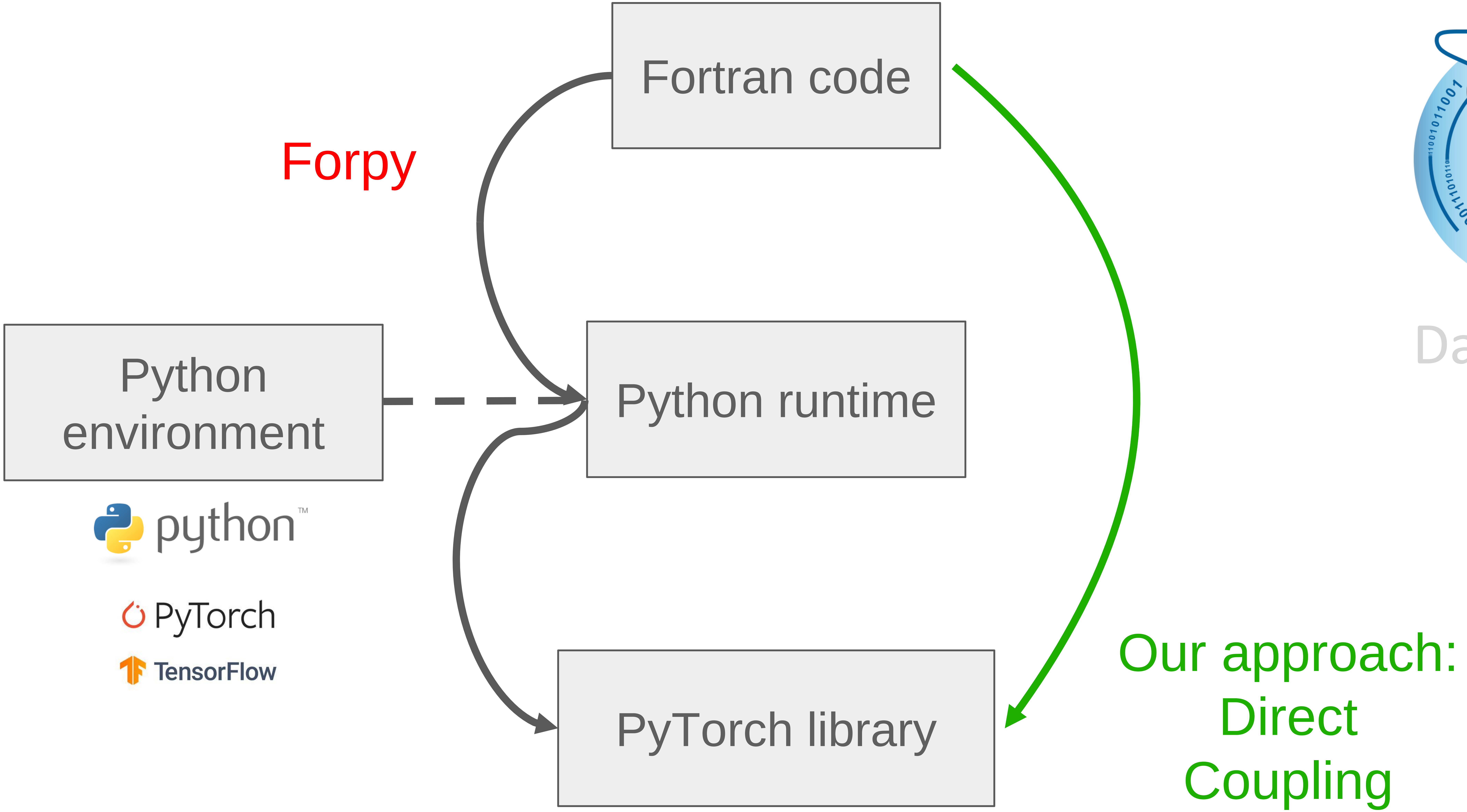
Model of an idealized Moist Atmosphere (MiMA)



DataWave

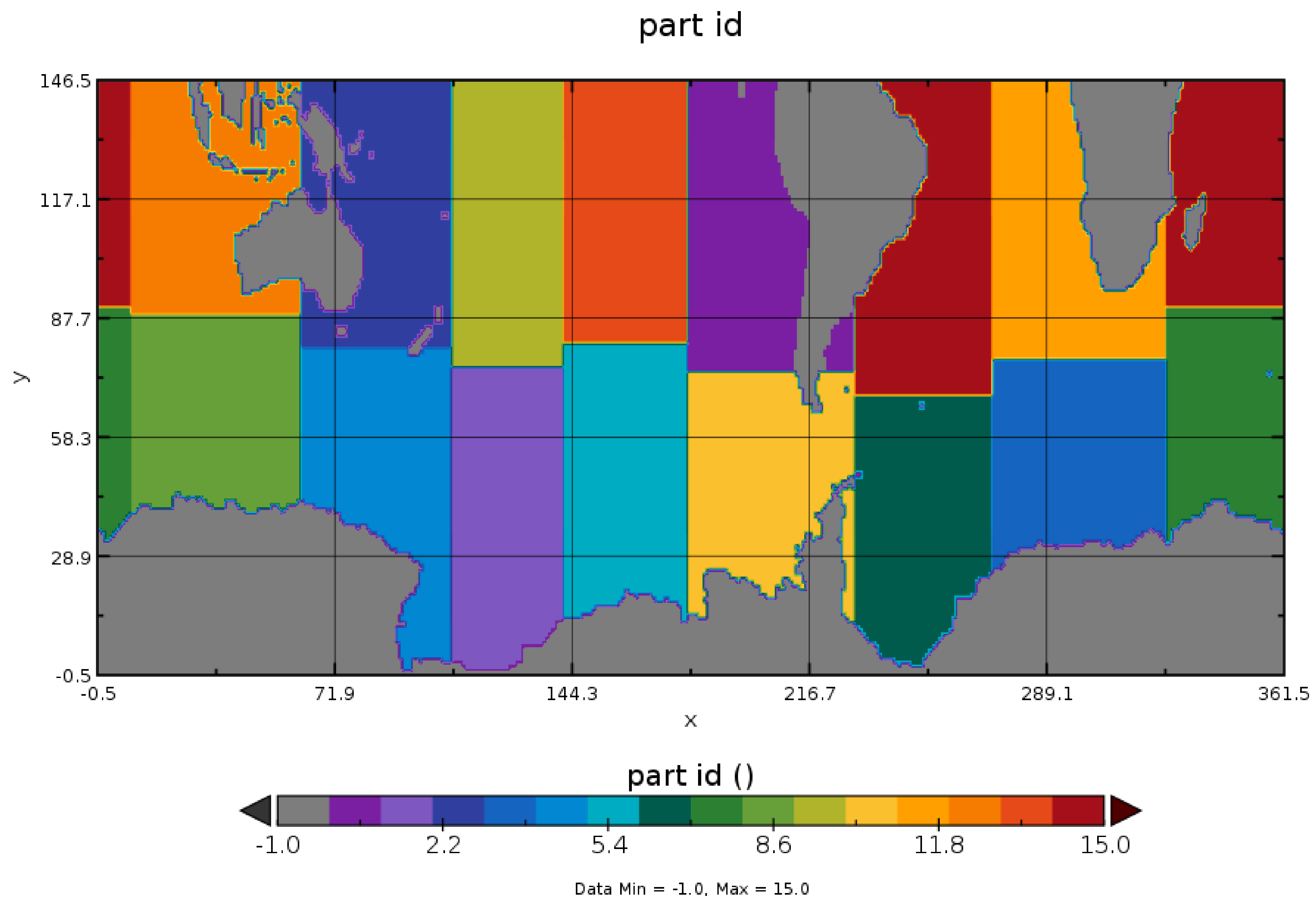
Challenges:

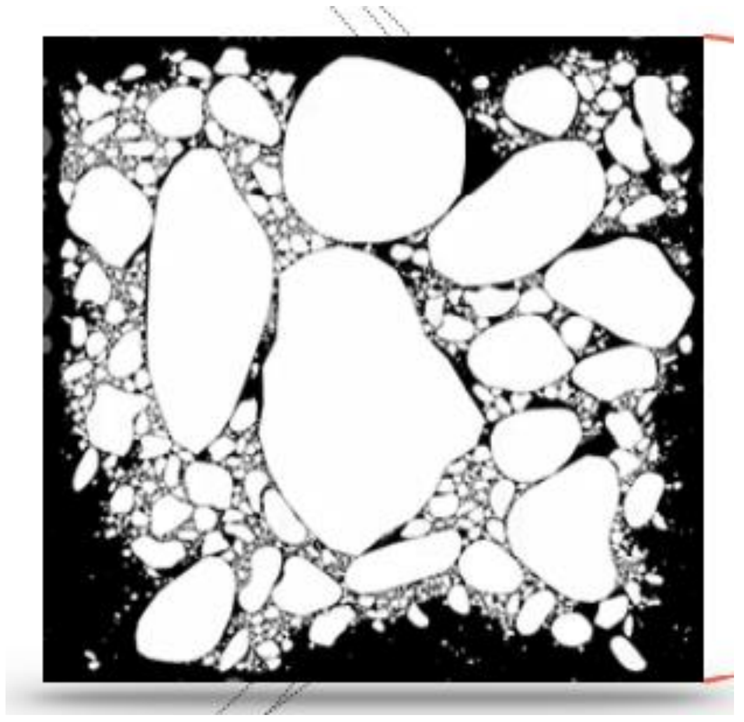
- fast inter-language interoperation (Python-Fortran)
- Advection (horizontal propagation) and its costs



DataWave

https://github.com/Cambridge-ICCS/fortran-pytorch-lib

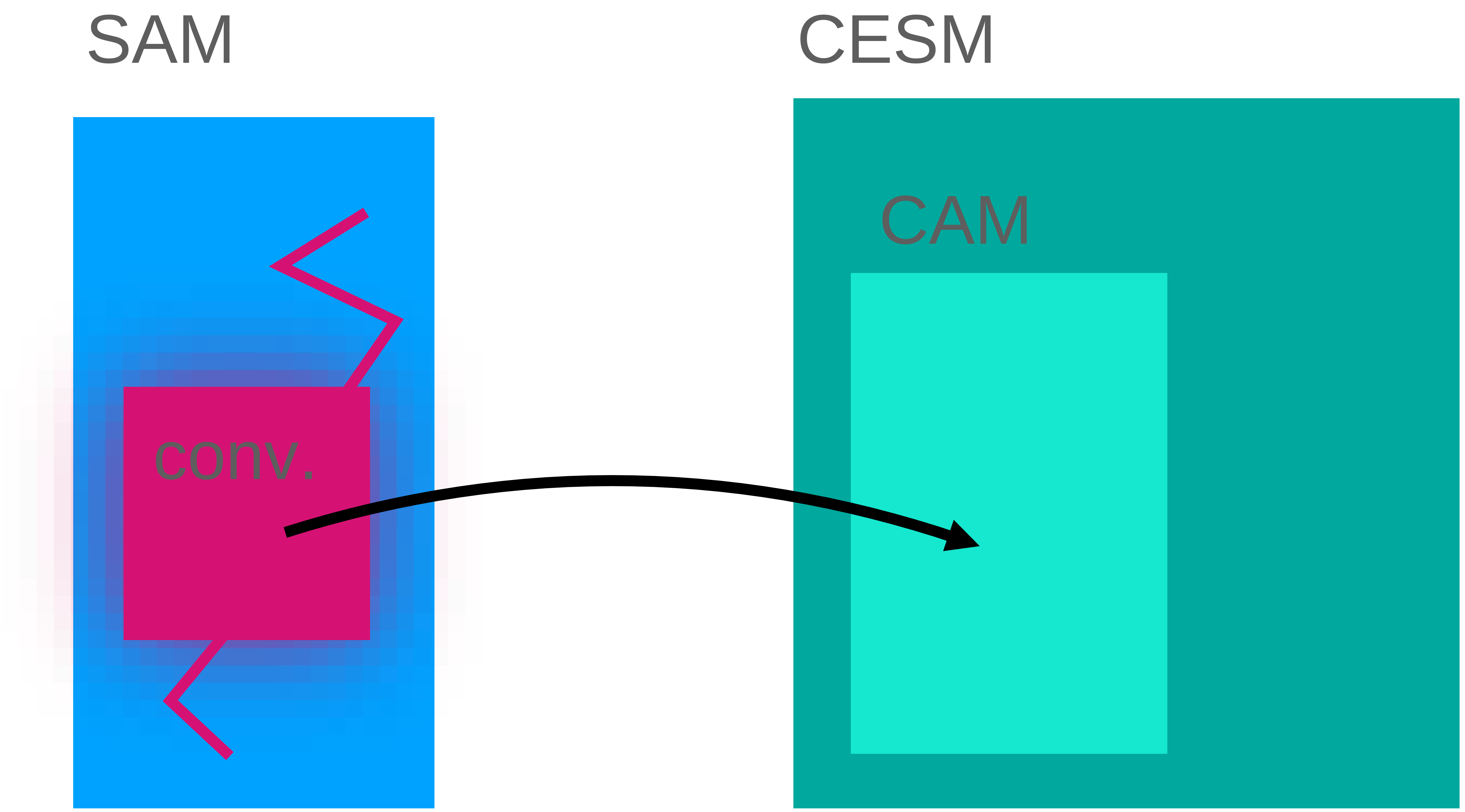




SASIP

- Data and task parallelisation
- Minimise data write time to improve performance
- Pre-computing land-mask in grid partitioning

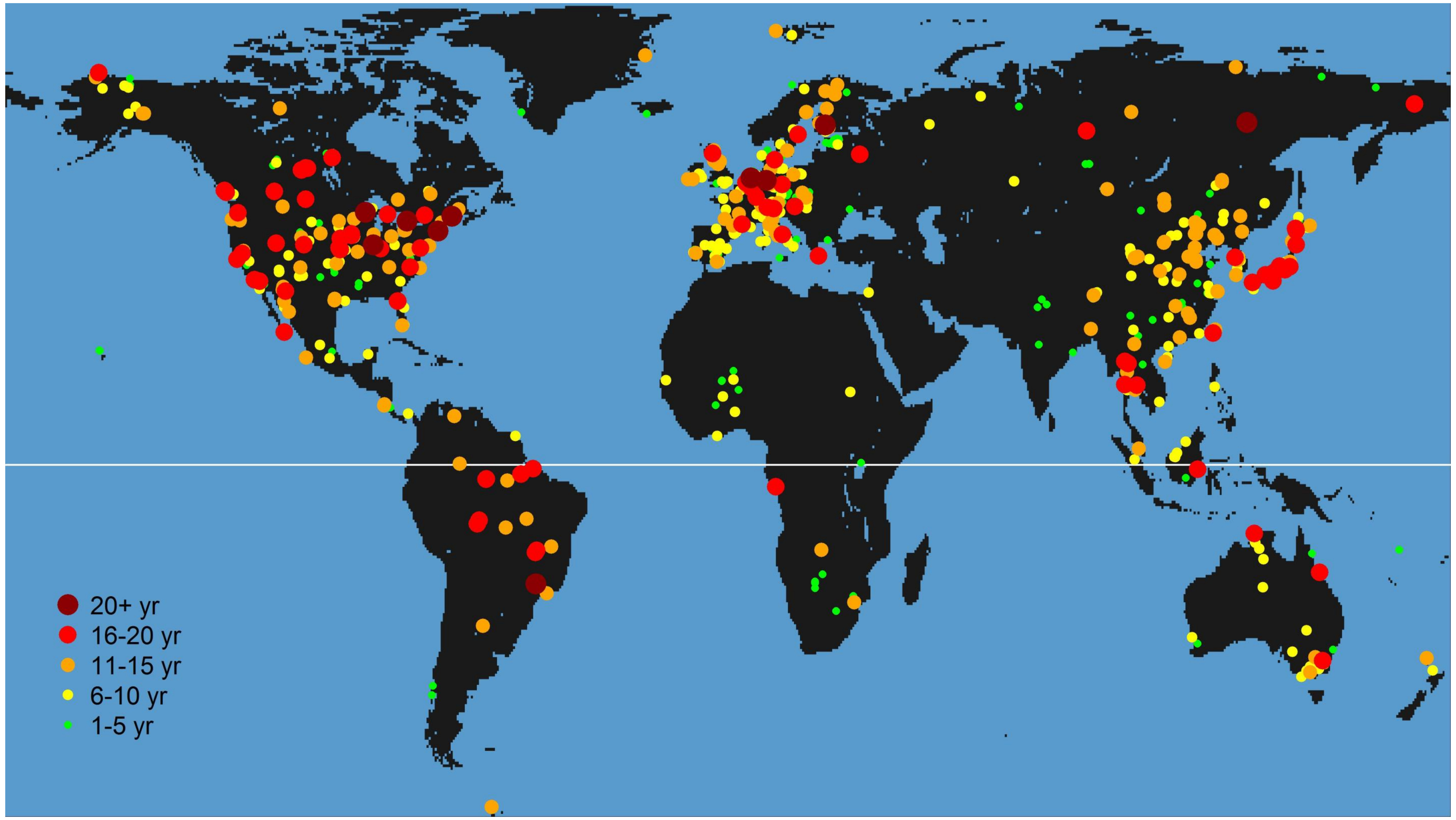
Redeploying Convection Parameterization



- Inputs use different physical properties …
- Need to ensure results are "correct"

FLUXNET

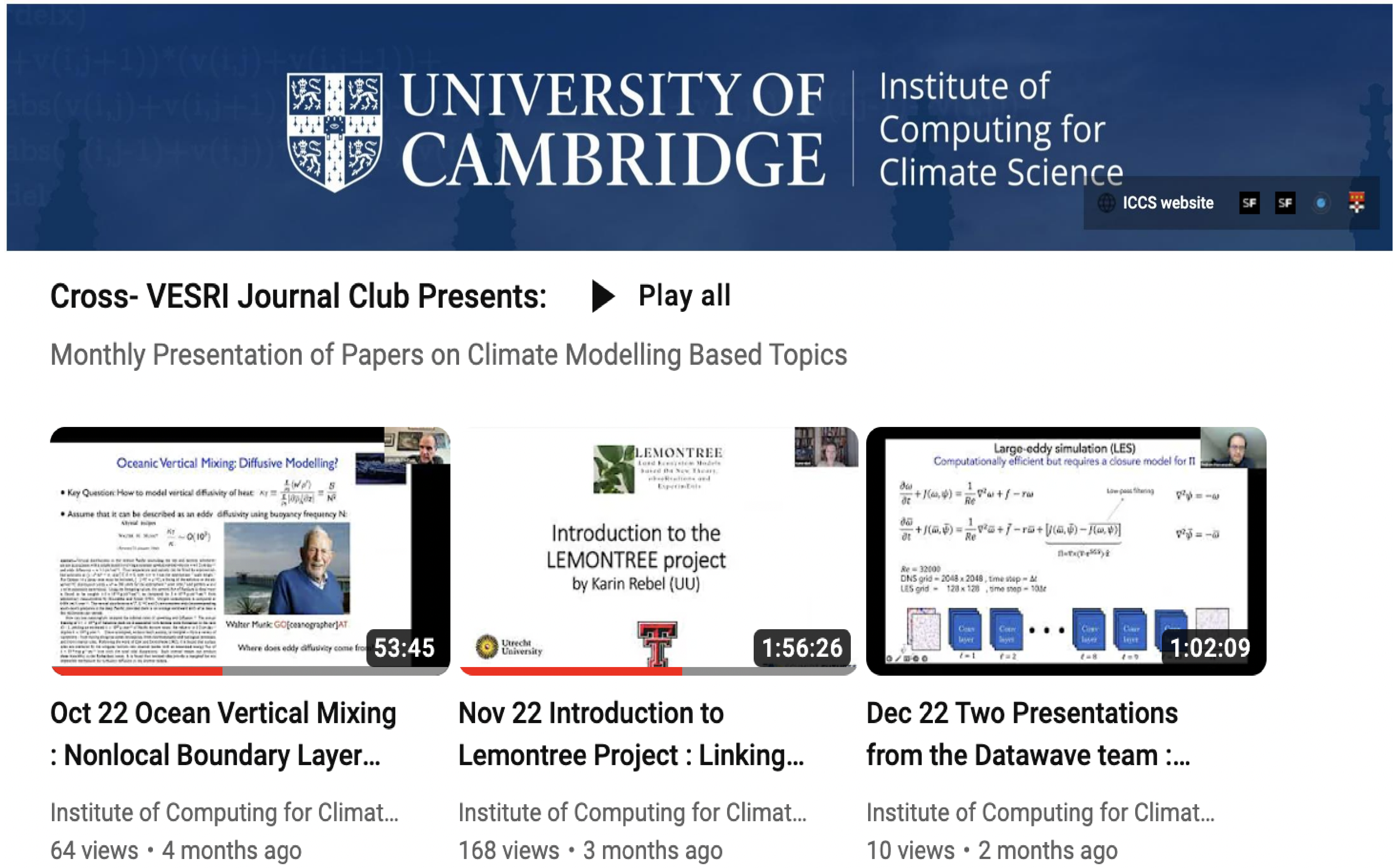
A Global Network

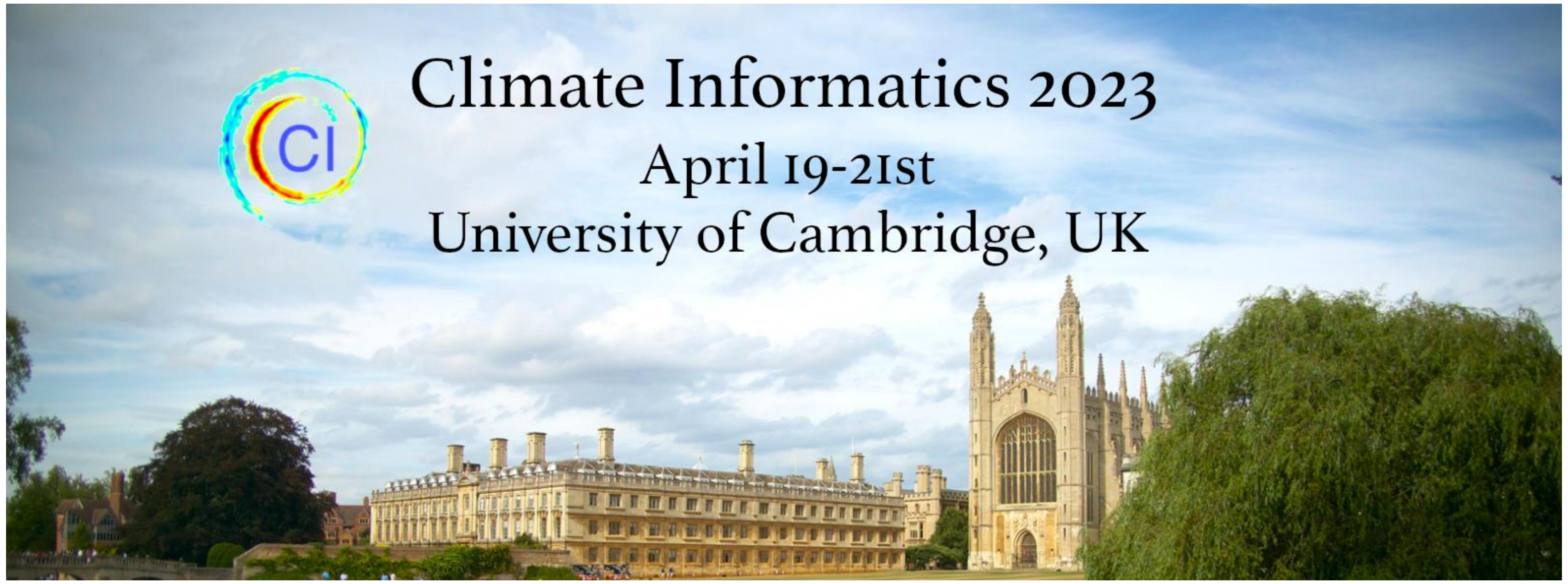


LEMONTREE

- Measure carbon, water, energy flux between biosphere and atmosphere
- FLUXNET 2015, >1000 sites processed, used in >400 studies
- 8 years un-processed largely due to software engineering issues and lack of support

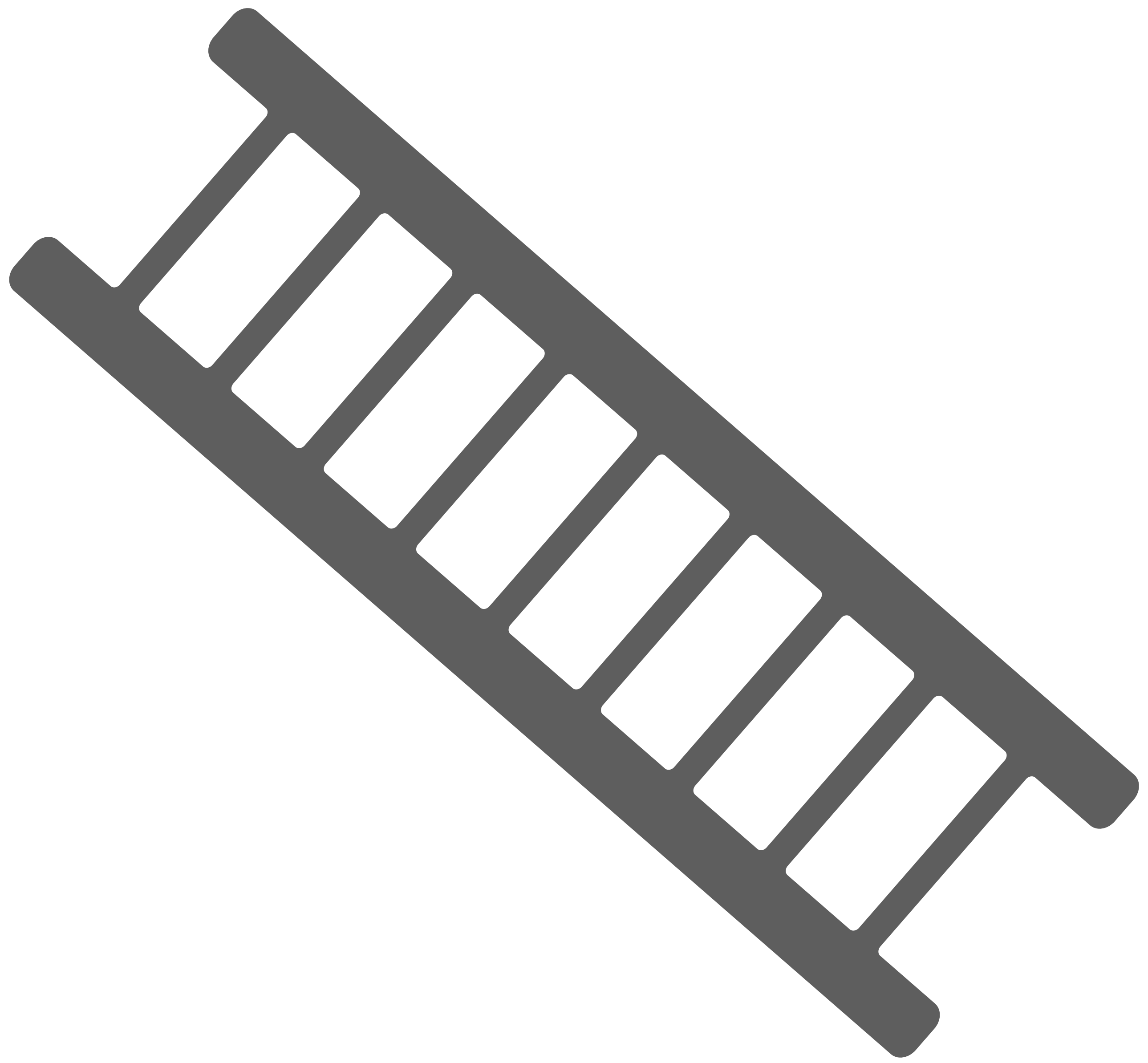
Community activities





Summary and parallels with ExaTEPP

- ICCS is a domain specific RSE group providing international support
- Provides a balance of climbing up and down the computational ladder



Institute of
Computing for
Climate Science