

High Performance Computing for Weather and Climate (HPC4WC)

Content: Introduction

Lecturer: Oliver Fuhrer

Block course 701-1270-00L

Summer 2023

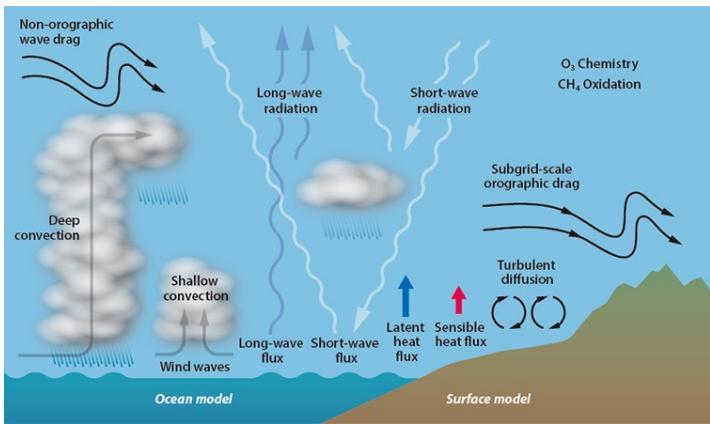


Learning goals

- Understand why weather and climate simulation requires high-performance computing (HPC)
- Understand why stencil computations are a key algorithmic motif of weather and climate models
- Understand a simple stencil program:
higher-order monotonic diffusion (Xue 2000, MWR)

Modeling the Earth system

Physical understanding



Governing equations (e.g. atmosphere)

$$\frac{d}{dt} \mathbf{v} = -2\Omega \times \mathbf{v} - \frac{1}{\rho} \nabla_3 p + \mathbf{g} + \mathbf{F} \quad \text{Conservation of momentum (Navier-Stokes)}$$

$$C_v \frac{d}{dt} (\rho q) + p \frac{d}{dt} \left(\frac{1}{\rho} \right) = J \quad \text{Conservation of energy (1st Law of Thermodynamics)}$$

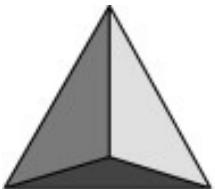
$$\frac{\partial}{\partial t} (\rho) = -\nabla_3 \cdot (\rho \mathbf{v}) \quad \text{Conservation of air mass}$$

$$\frac{\partial}{\partial t} = -\nabla_3 \cdot (\rho \mathbf{v} q) + \rho (E - C) \quad \text{Continuity of water vapor mass}$$

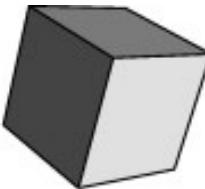
$$p = \rho R T \quad \text{Equation of state (Ideal gas law)}$$

Variables: $\{\mathbf{v}, p, T, \rho, q\}$

Grids on a sphere



Tetrahedron



Hexahedron



Octahedron

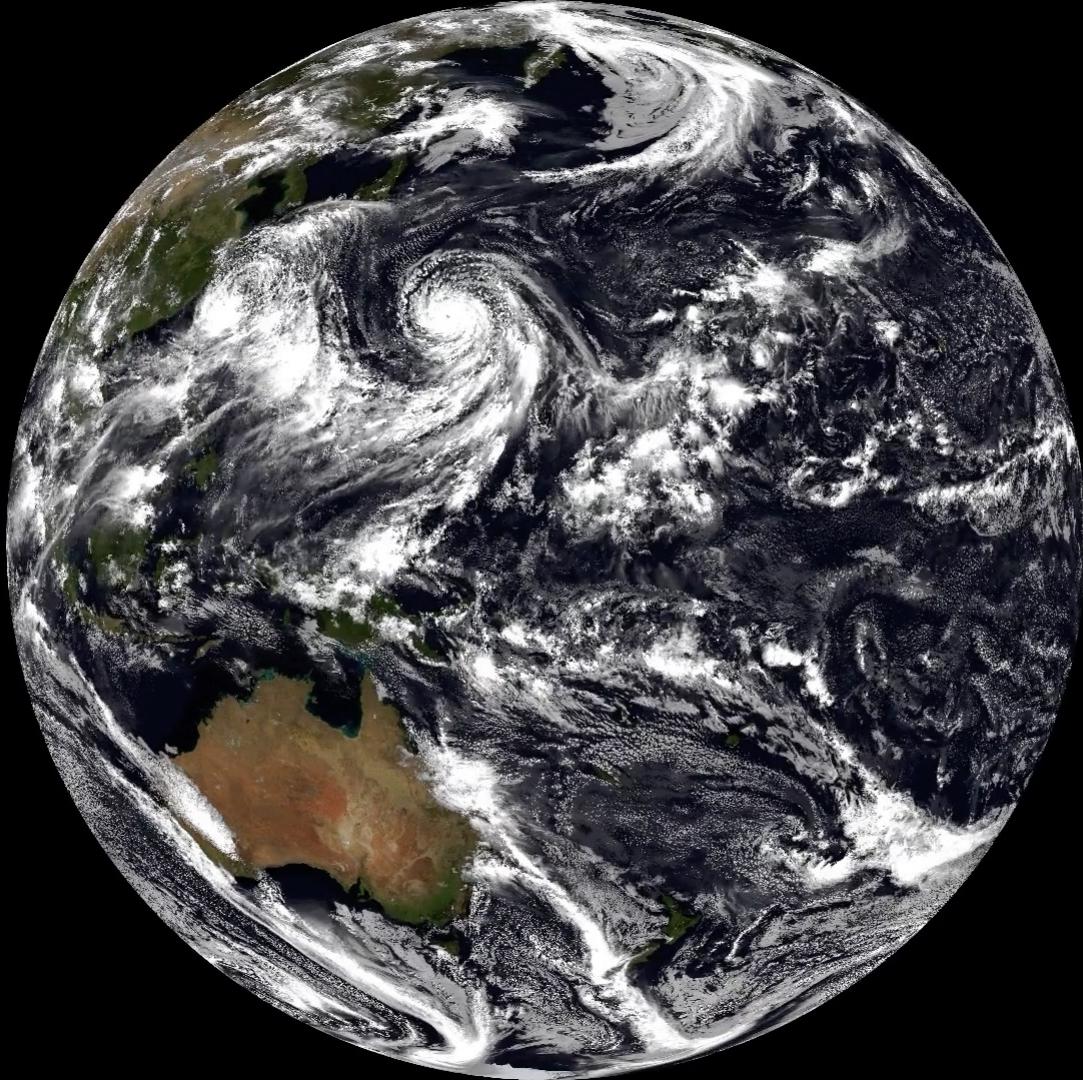


Dodecahedron



Icosahedron



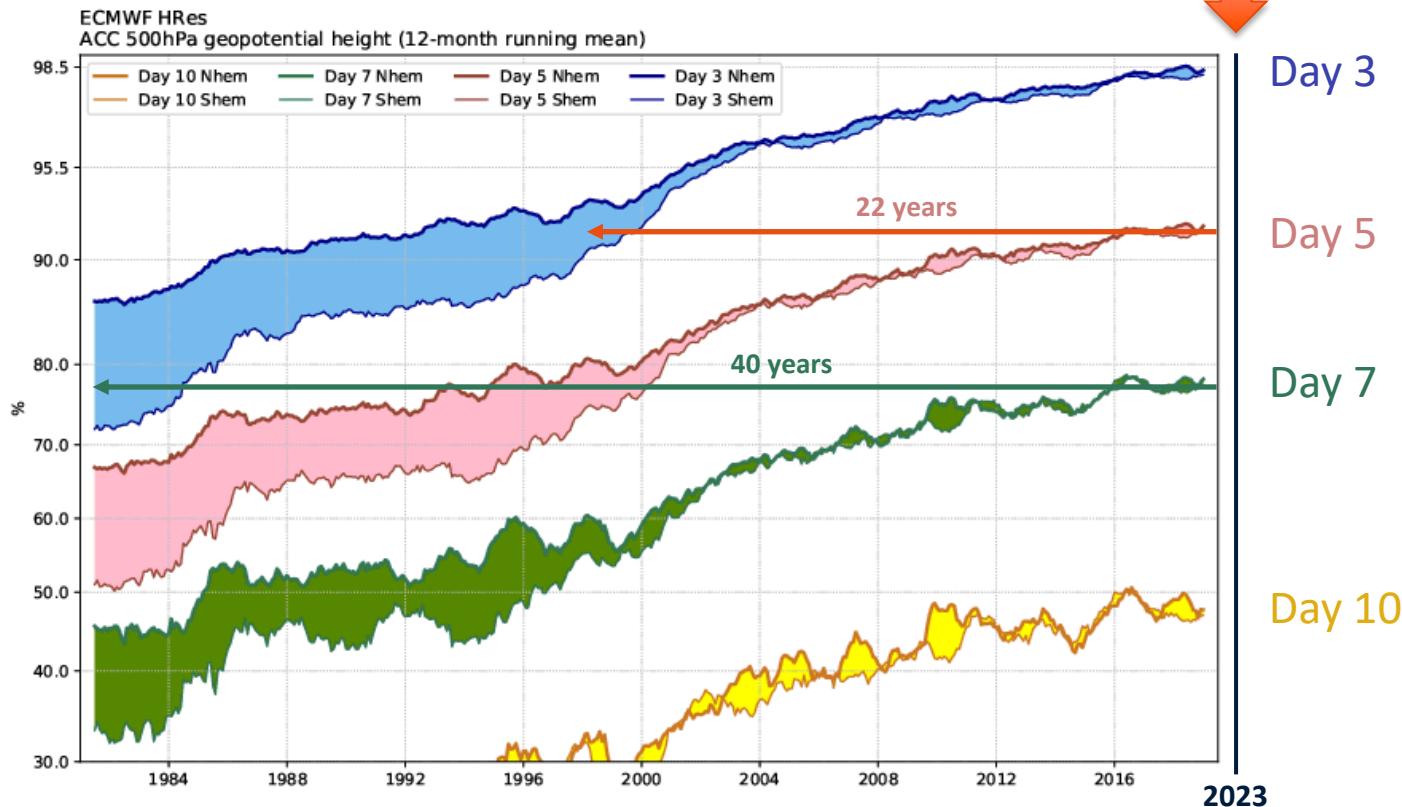


2016-08-11 18:00Z
258 Forecast Hours
FV3 3km

Visualization
Xi Chen@FV3 team
[Introduction](#) 5

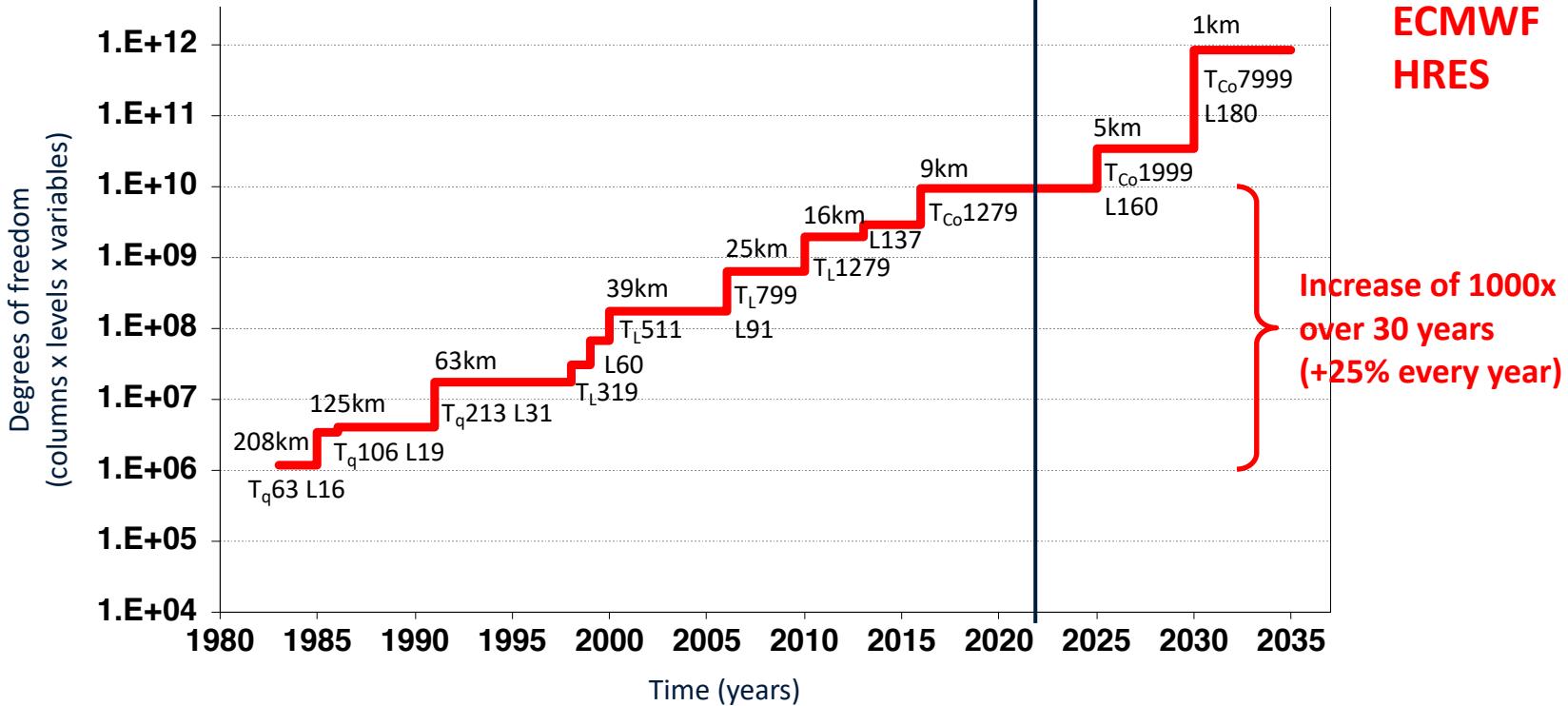
Forecast skill over time

You are here!



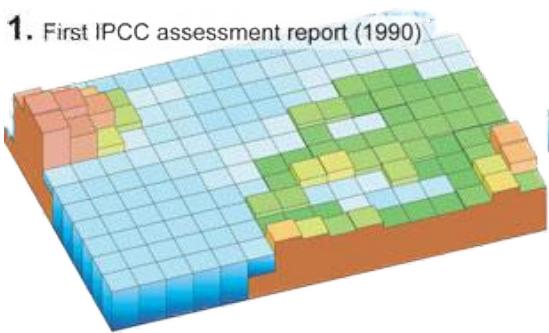
Grid resolution drives skill

You are here!

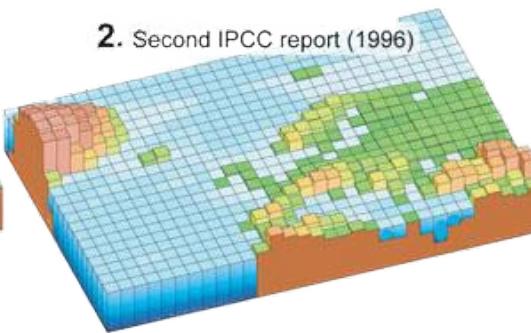


Grid resolution in the IPCC

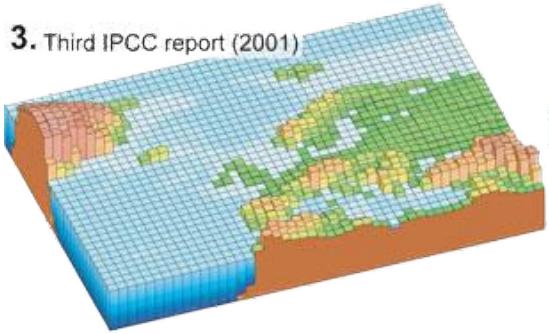
1. First IPCC assessment report (1990)



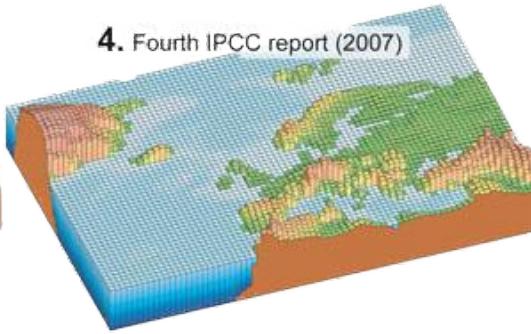
2. Second IPCC report (1996)



3. Third IPCC report (2001)



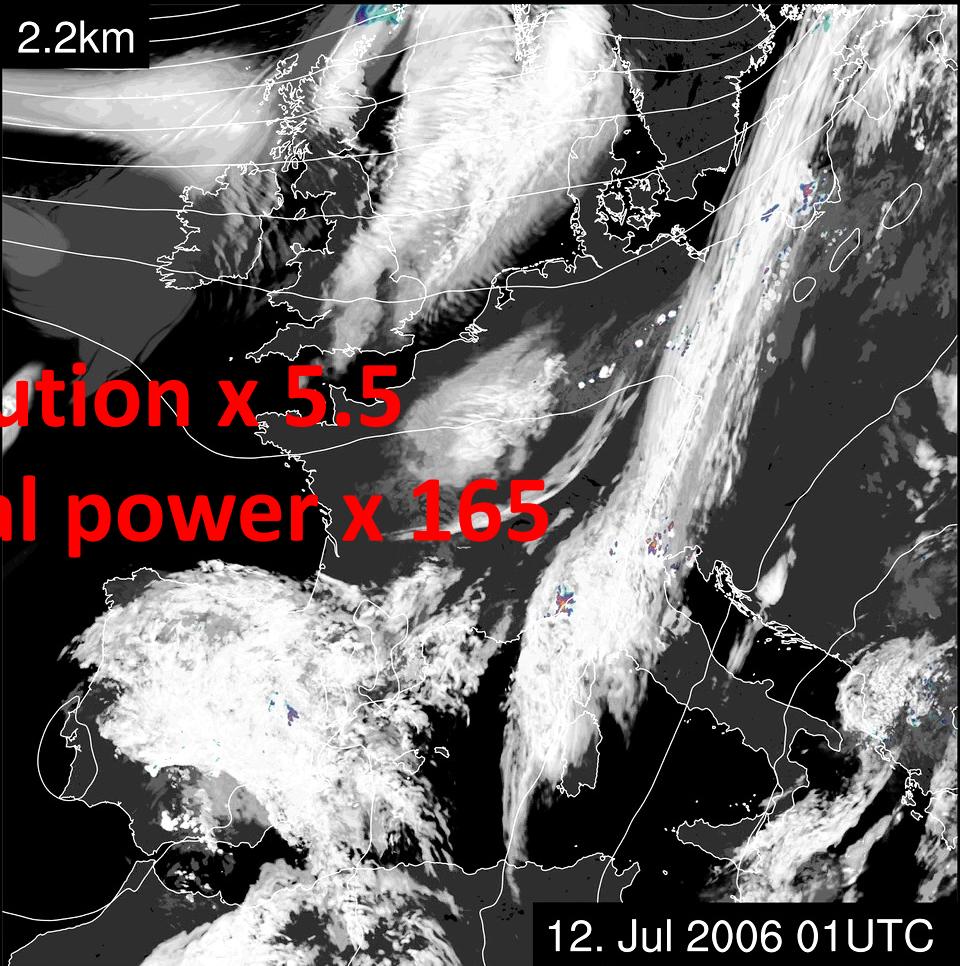
4. Fourth IPCC report (2007)



12km



2.2km

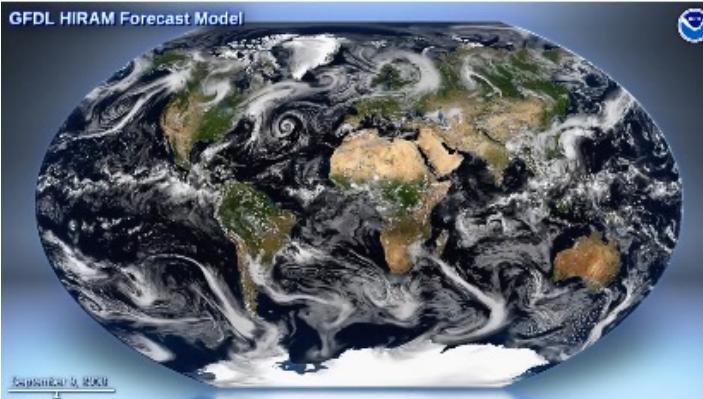
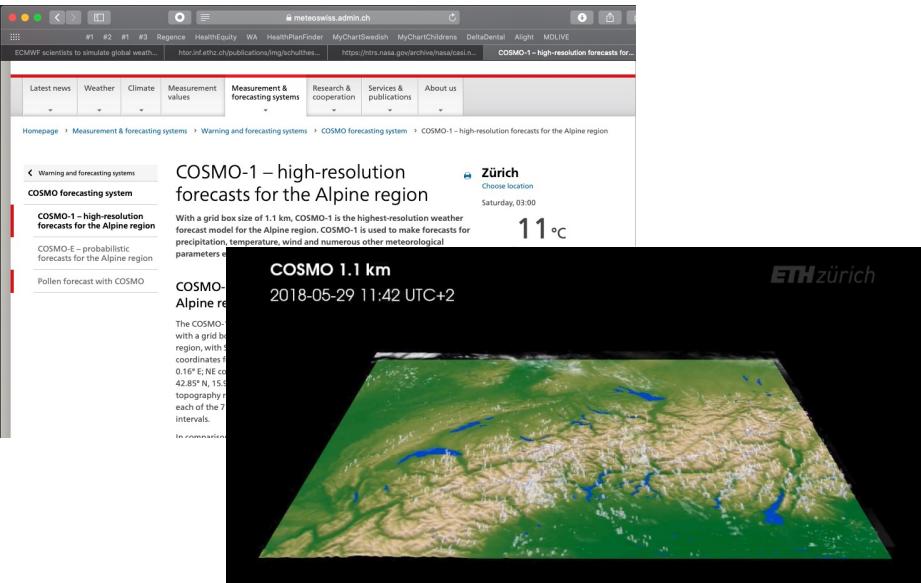


Grid resolution x 5.5
Computational power x 165

12. Jul 2006 01UTC

Example applications

- Swiss national weather forecast (COSMO-1E)
 $1152 \times 774 \times 80$ gridpoints
 $\Delta x = 1.1$ km
 $\Delta t = 10$ s
11 members
80x faster than real time (0.2 SYPD)
- Global climate model with 3 km resolution (DYAMOND)
 $57 \times 10^6 \times 80$ gridpoints
 $\Delta x = 3.0$ km
 $\Delta t = 9$ s
1000x faster than real time (3 SYPD)



Why HPC?

- Swiss national weather forecast

([COSMO-1](#))

$1152 \times 774 \times 80$ gridpoints

$\Delta x = 1.1$ km

$\Delta t = 10$ s

11 members

80x faster than real time



Intel Xeon E5-2690 v3
@2.6 Ghz, 135 W

~ 8'250 CPUs

~ 1100 kW (= 1400 households)

- Global climate model with 3 km resolution ([DYAMOND](#))

$57 \times 10^6 \times 80$ gridpoints

$\Delta x = 3.0$ km

$\Delta t = 9$ s

~~1000x faster than real time~~

~ 750'000 CPUs

~ 100 MW (= 10% of Gösgen)

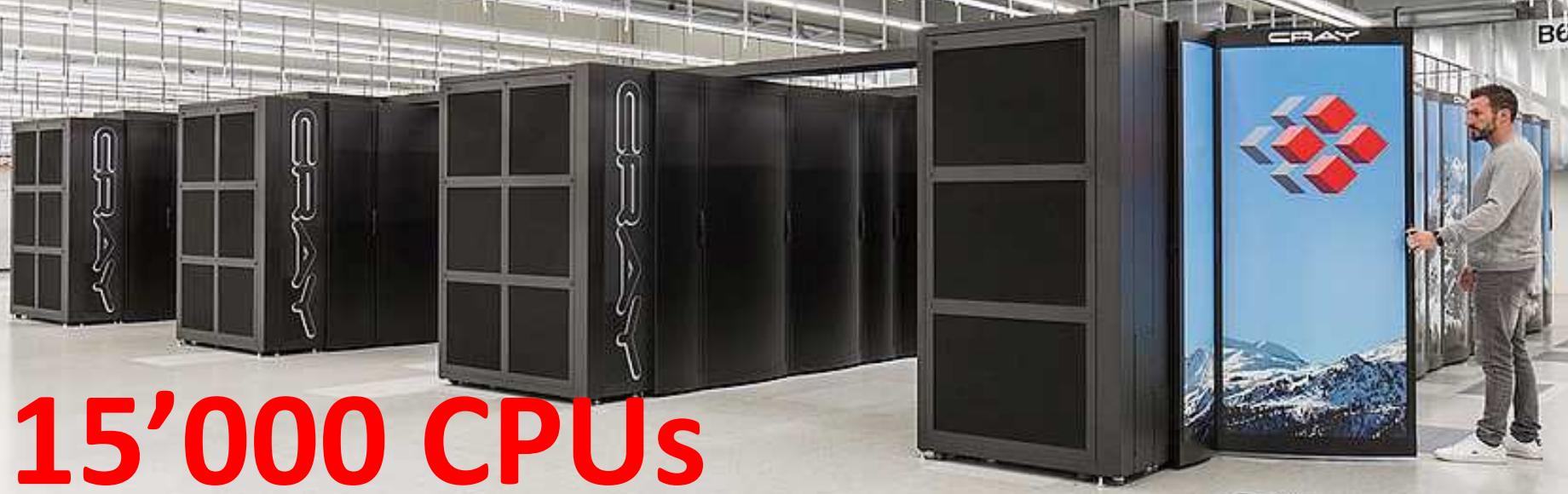
Currently only 100x feasible!

~130 CPUs

(only sufficient for one COSMO-1E member)



C

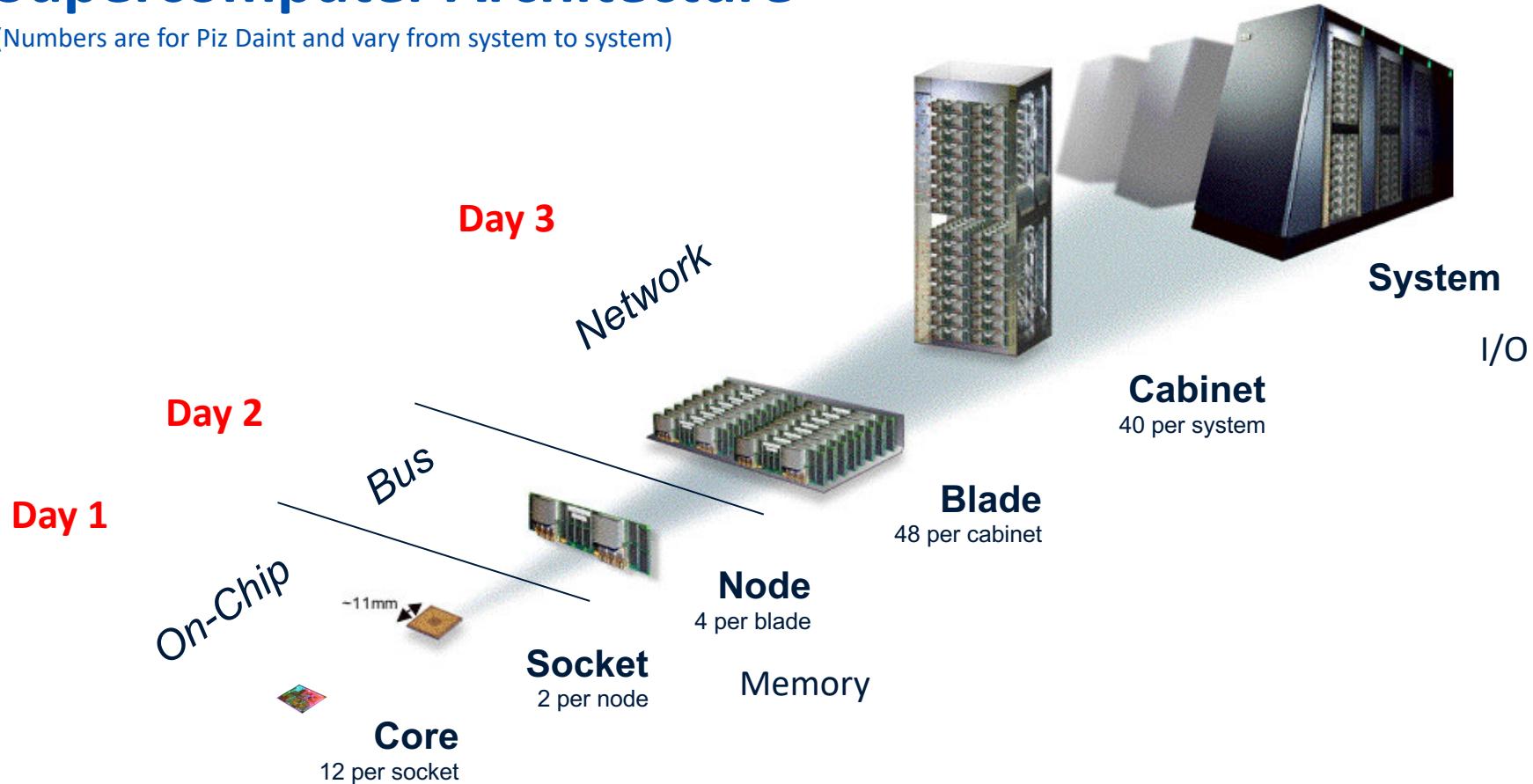


15'000 CPUs

(~ 15 x more dense!)

Supercomputer Architecture

(Numbers are for Piz Daint and vary from system to system)



“ *High Performance Computing* is the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business.

Lab Exercises

01-roofline-model.ipynb

- Learn about performance metrics and how to compute theoretical peak values.
- Learn about arithmetic intensity and performance limiters.

02-stencil-program.ipynb

- Determine arithmetic intensity of a stencil program.
- Apply a performance profiling tool to gain insight into performance.
- Show limitations of the von Neumann model for understanding performance.

03-caches-data-locality.ipynb

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higher-order monotonic diffusion (Xue 2000, MWR)

Higher-order diffusion (Xue 2000, MWR)

- Atmospheric and ocean models often need some form of numerical filtering to control small-scale noise.
- Xue 2000 (Monthly Weather Review) published a class of higher-order monotonic filters that are frequently used.
- We will focus on the 4th-order non-monotonic diffusion for this course.

2853

XUE

AUGUST 2000

High-Order Monotonic Numerical Diffusion and Smoothing

MING XUE

Center for Analysis and Prediction of Storms, University of Oklahoma, Norman, Oklahoma

(Manuscript received 28 May 1999, in final form 17 September 1999)

ABSTRACT

High-order numerical diffusion is commonly used in numerical models to provide scale selective control over small-scale noise. Conventional high-order schemes have undesirable side effects, however; they can introduce noise themselves. Two types of monotonic high-order diffusion schemes are proposed. One is based on flux correction/limiting on the corrective fluxes, which is the difference between a high-order (fourth order and above) diffusion scheme and a lower-order (typically second order) one. Overshooting and undershooting found in the solutions of higher-order diffusions near sharp gradients are prevented, while the highly selective property of damping is retained.

The second simpler (flux limited) scheme simply ensures that the diffusive fluxes are always downgradient; otherwise, the fluxes are set to zero. This much simpler scheme yields as good a solution in 1D cases as and better solutions in 2D than the one using the first more elaborate flux limiter. The scheme also preserves monotonicity in the solutions and is computational much more efficient.

The simple flux-limited fourth- and sixth-order diffusion schemes are also applied to thermal bubble convection. It is shown that overshooting and undershooting are consistently smaller when the flux-limited version of the high-order diffusion is used, no matter whether the advection scheme is monotonic or not. This conclusion applies to both scalar and momentum fields. Higher-order monotonic diffusion works better and even more so when used together with monotonic advection.

1. Introduction

Most numerical models employ numerical diffusion or computational mixing to control small-scale (near two grid intervals in wavelength) noise that can arise from numerical dispersion, nonlinear instability, discontinuous physical processes, and external forcing. Such diffusion cannot always be substituted for by physical parameterization, whose

resents other processes or sources. The last term on the right-hand side (rhs) is the added diffusion term and n ($=0, 2, 4, 6, \dots$) denotes the order. Here α_n is called diffusion coefficient. Diffusion or smoothing can also be introduced by periodically applying a spatial filter or smoother to the predicted field (e.g., Shapiro 1970, 1975). Its effect is often equivalent to applying diffusion in the prognostic equation for a period of time.

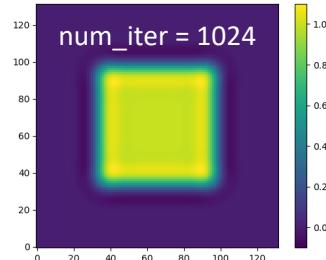
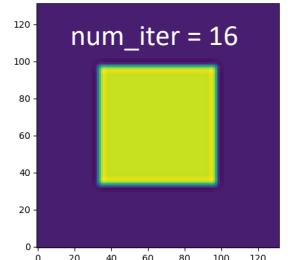
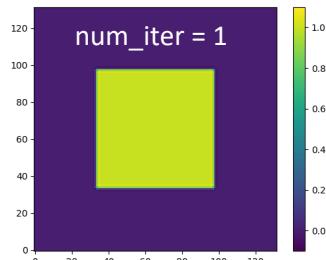
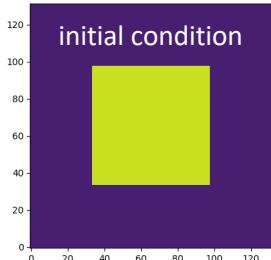
Second- and fourth-order formulations are most com-

Governing equations

High-order monotonic diffusion
(see paper)

Simplifications (see paper)

- ignore other processes ($S=0$)
- 4th-order ($n=4$)
- without limiter



$$\frac{\partial \phi}{\partial t} = S + (-1)^{n/2+1} \alpha_n \nabla^n \phi, \quad (1)$$

$$S = 0 \quad n = 4 \quad \text{horizontal}$$

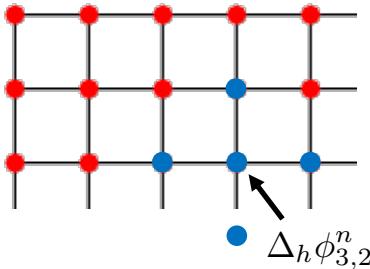
$$\begin{aligned} \frac{\partial \phi}{\partial t} &= -\alpha_4 \nabla_h^4 \phi \\ &= -\alpha_4 \Delta_h^2 \phi \quad \Delta_h = \nabla_h^2 \end{aligned}$$

$$\boxed{\frac{\partial \phi}{\partial t} = -\alpha_4 \Delta_h (\Delta_h \phi)}$$

Discretization: Finite difference method (FDM)

Computational grid

Store values at gridpoints (i,j)



$$x_{i,j} = i \Delta x \quad y_{i,j} = j \Delta y$$

$$t^n = n \Delta t$$

$$\phi_{i,j}^n = \phi(x_{i,j}, y_{i,j}, t^n)$$

Spatial discretization

2nd-order centered

$$\Delta_h \phi_{i,j}^n \approx (-4 \phi_{i,j}^n + \phi_{i-1,j}^n + \phi_{i+1,j}^n + \phi_{i,j-1}^n + \phi_{i,j+1}^n) / \Delta x^2$$

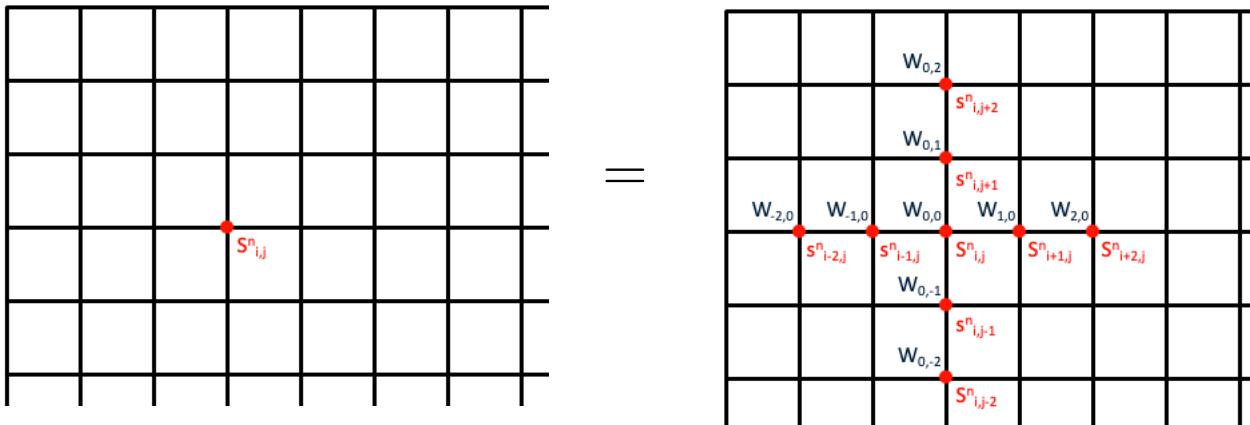
Time discretization

1st-order forward (Euler)

$$\partial_t \phi_{i,j}^n \approx (\phi_{i,j}^{n+1} - \phi_{i,j}^n) / \Delta t$$

Stencil computation (5x5, sparse)

$$s_{i,j}^{n+1} = \sum_{i_{\text{rel}}, j_{\text{rel}}} w_{i_{\text{rel}}, j_{\text{rel}}} s_{i+i_{\text{rel}}, j+j_{\text{rel}}}^n$$



weighted sum of grid values
compact neighborhood
same pattern ∀ gridpoints

“ A *stencil computation* is an algorithmic motif where the value at a certain grid point is computed from a compact neighborhood of gridpoints in it’s vicinity on the computational grid using the same pattern for every gridpoint. ”

Stencil program

$$\frac{\partial \phi}{\partial t} = -\alpha_4 \Delta_h (\Delta_h \phi)$$



Discretization

$$\Delta_h \phi_{i,j}^n \approx (-4 \phi_{i,j}^n + \phi_{i-1,j}^n + \phi_{i+1,j}^n + \phi_{i,j-1}^n + \phi_{i,j+1}^n) / \Delta x^2$$

$$\partial_t \phi_{i,j}^n \approx (\phi_{i,j}^{n+1} - \phi_{i,j}^n) / \Delta t$$

$$\alpha = \alpha_4 \frac{\Delta t}{\Delta x^2}$$

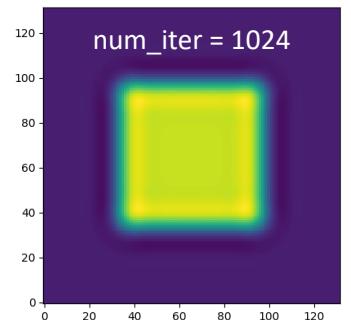
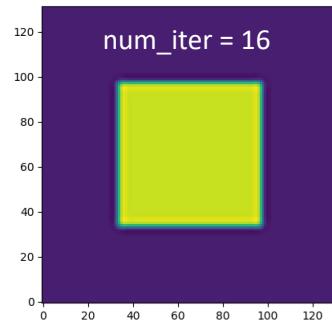
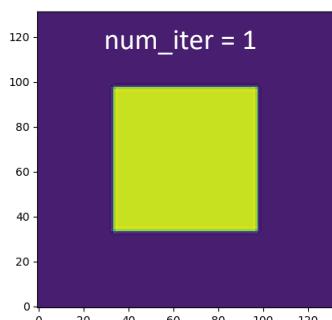
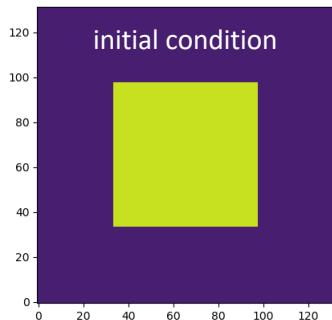


Implementation

```
do num_iter:  
    tmp = lap(in)  
    out = lap(tmp)  
    out = in - alpha * out  
    swap(in, out)
```

Structure of stencil_2d.F90 / stencil_2d.py

```
tmpi,j,k = lap(ini,j,k) = -4 ini,j,k + ini-1,j,k + ini+1,j,k + ini,j-1,k + ini,j+1,k
outi,j,k = lap(tmpi,j,k) = -4 tmpi,j,k + tmpi-1,j,k + tmpi+1,j,k + tmpi,j-1,k + tmpi,j+1,k
outi,j,k = ini,j,k - α outi,j,k
if iter < num_iter : swap(in,out)
```



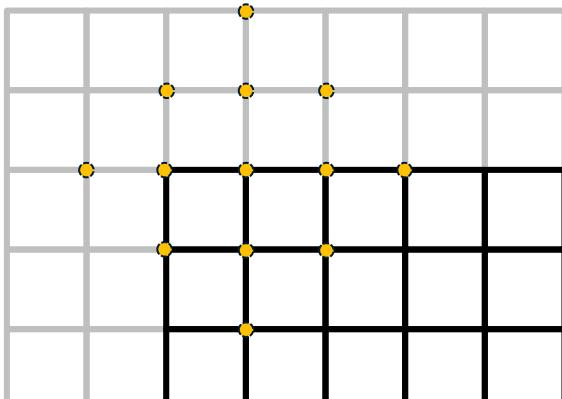
Halo points

halo_update(in)

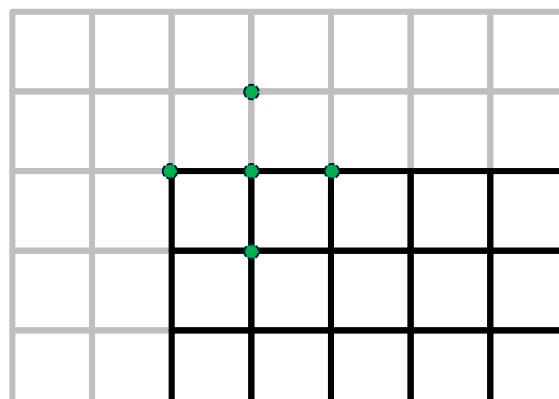
$$\underline{\text{tmp}_{i,j,k}} = \text{lap}(\underline{\text{in}_{i,j,k}}) = -4\underline{\text{in}_{i,j,k}} + \underline{\text{in}_{i-1,j,k}} + \underline{\text{in}_{i+1,j,k}} + \underline{\text{in}_{i,j-1,k}} + \underline{\text{in}_{i,j+1,k}}$$

$$\underline{\text{out}_{i,j,k}} = \text{lap}(\underline{\text{tmp}_{i,j,k}}) = -4\underline{\text{tmp}_{i,j,k}} + \underline{\text{tmp}_{i-1,j,k}} + \underline{\text{tmp}_{i+1,j,k}} + \underline{\text{tmp}_{i,j-1,k}} + \underline{\text{tmp}_{i,j+1,k}}$$

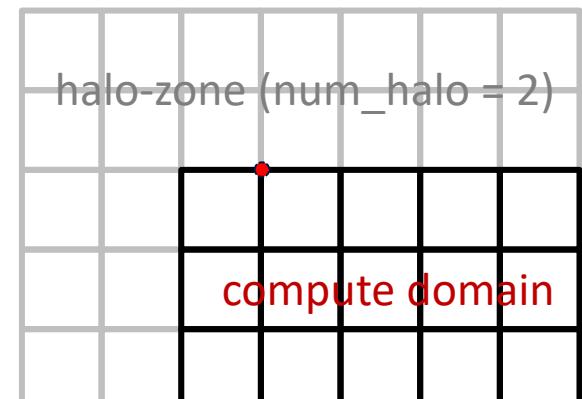
$$\text{out}_{i,j,k} = \text{in}_{i,j,k} - \alpha \underline{\text{out}_{i,j,k}}$$



in(i,j,1)



tmp(i,j,1)

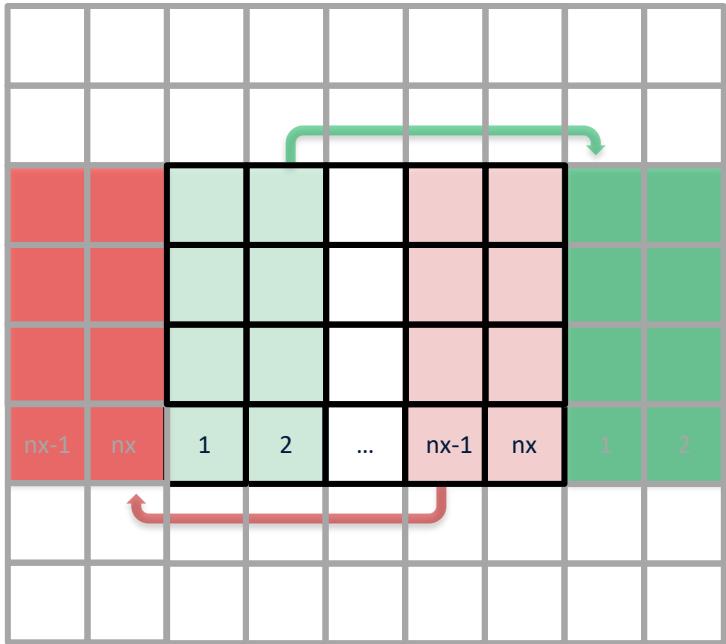


out(i,j,1)

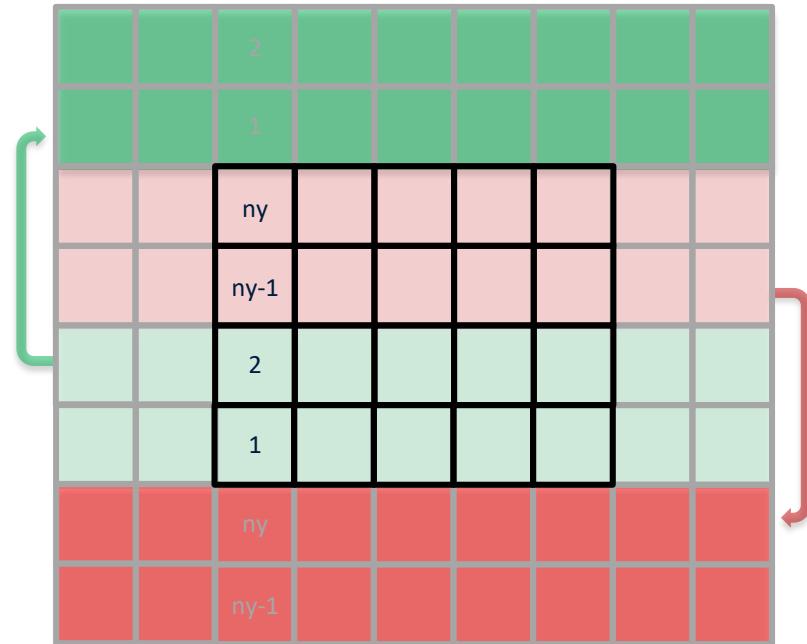
halo-zone (num_halo = 2)

compute domain

Halo update (periodic)



`field(nx + 2 * num_halo, ny + 2 * num_halo, nz)`



Summary

- Spatial resolution drives required computational power $1/\Delta x^3$, this is why we need supercomputers for modeling weather and climate.
- While models use a myriad of different numerical techniques to solve the governing PDEs, the main algorithmic motif resulting from these methods are stencil computations.

Our course will **focus exclusively on stencil computations**, but the concepts are more general and transferable.

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