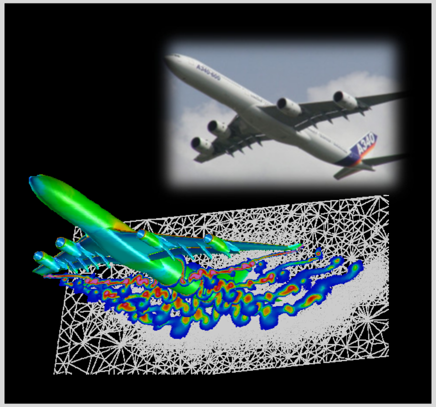

High Performance Computing

ADVANCED SCIENTIFIC COMPUTING

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SHORT LECTURE 12

Terrestrial Systems and Climate

November 18, 2019

Webinar

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

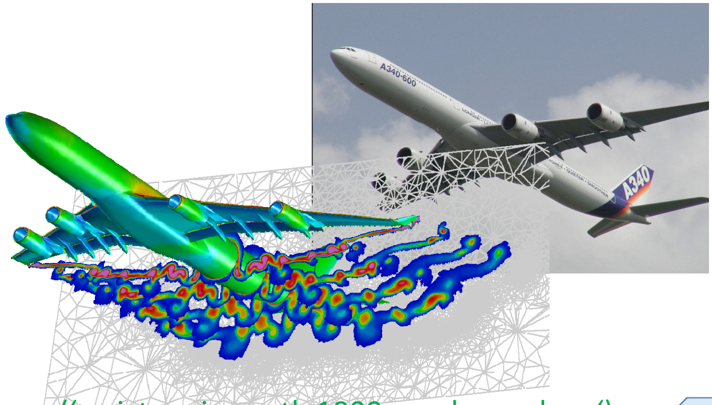
JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

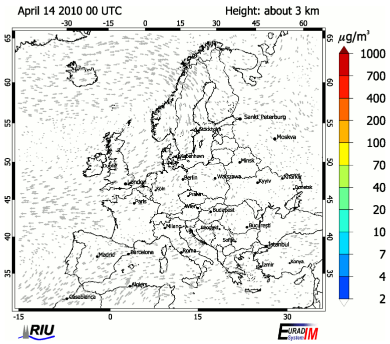
DEEP Projects

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

HAICU HELMHOLTZ ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Review of Short Lecture 11 – Scientific Visualization & Scalable Infrastructures





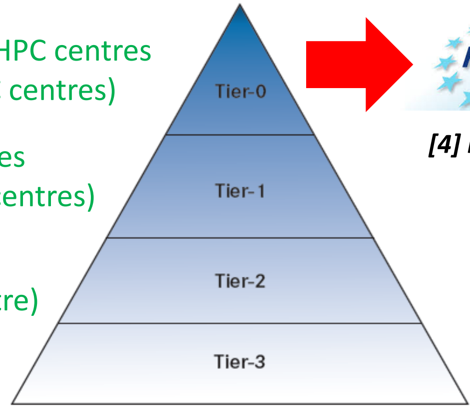
('a picture is worth 1000 ~~words~~ numbers')

Large-scale HPC centres
(e.g. EU HPC centres)

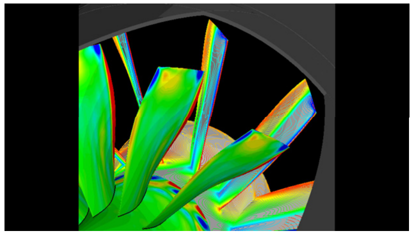
National HPC centres
(e.g. German HPC centres)

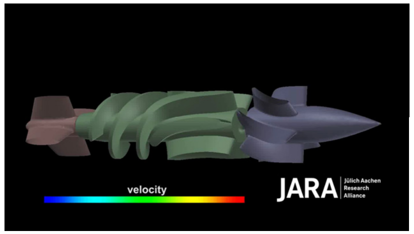
Topical and Regional HPC
Centres (e.g. climate centre)

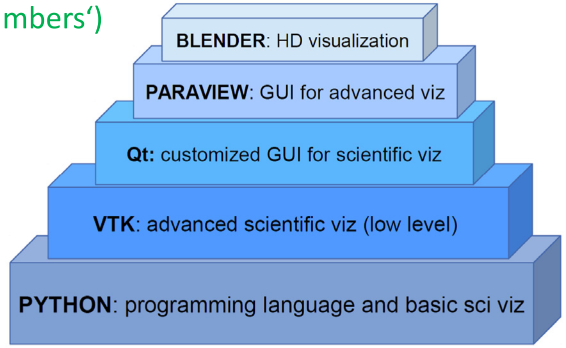
Servers and small clusters
(e.g. universities, institutes)



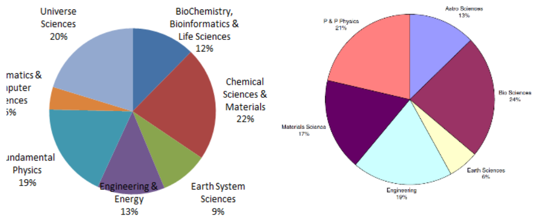
[4] PRACE RI



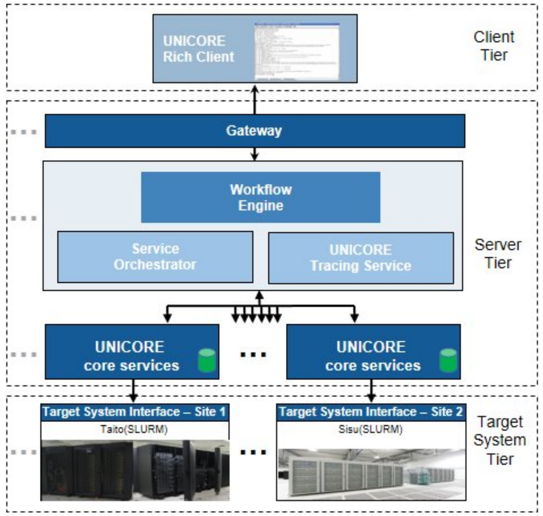




[1] CINECA – Scientific Visualization Training



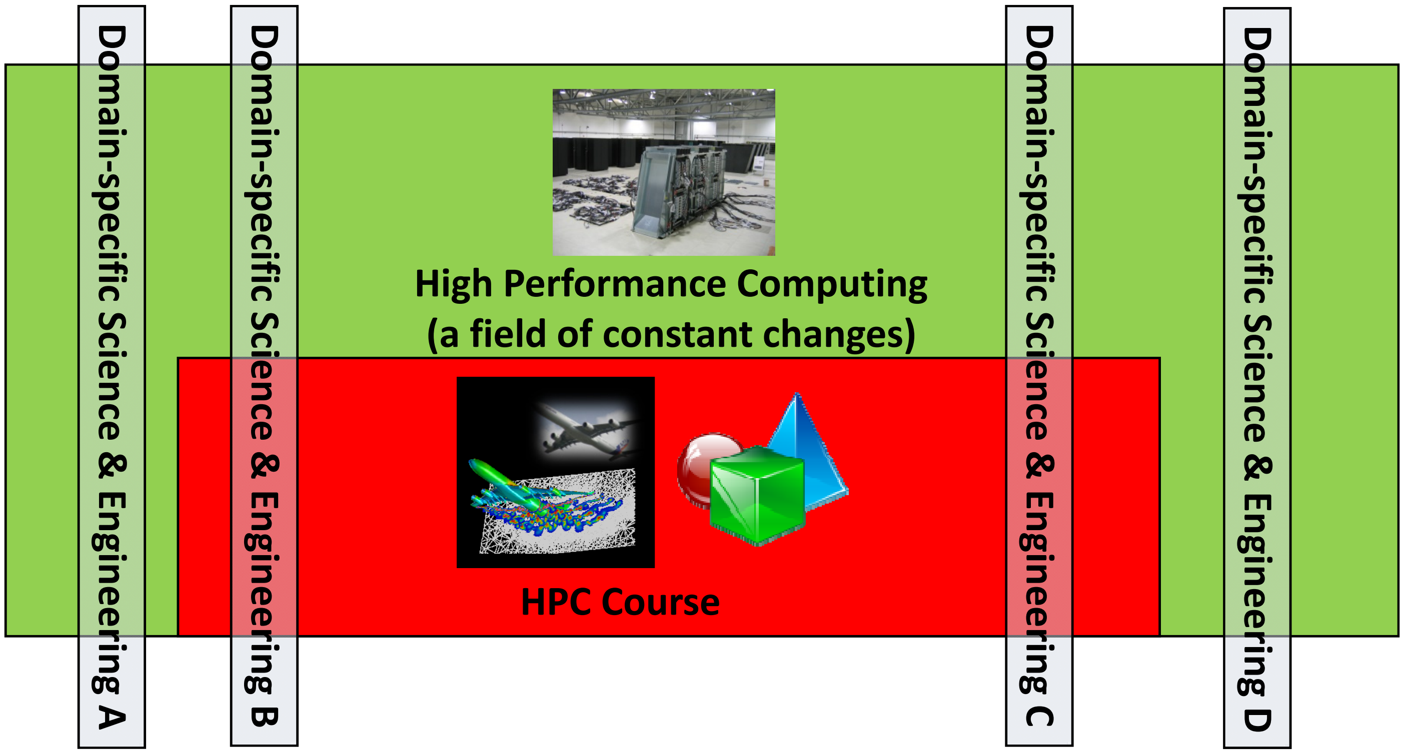
[3] M. Memon & M. Riedel et al., 'Scientific workflows applied to the coupling of a continuum (Elmer v8.3) and a discrete element (HiDEM v.1.0) ice dynamic model', 2019



[2] W. Gentzsch and M. Riedel et al., 'DEISA – Distributed European Infrastructure for Supercomputing Applications', Journal of Grid Computing, 2011

HPC-A[dvanced] Scientific Computing (cf. Prologue) – Second Part

- Consists of techniques for programming & using large-scale HPC Systems
  - Approach: Get a broad understanding what HPC is and what can be done
  - Goal: Train general HPC techniques and systems and selected details of domain-specific applications



Outline of the Course

1. High Performance Computing
2. Parallel Programming with MPI
3. Parallelization Fundamentals
4. Advanced MPI Techniques
5. Parallel Algorithms & Data Structures
6. Parallel Programming with OpenMP
7. Graphical Processing Units (GPUs)
8. Parallel & Scalable Machine & Deep Learning
9. Debugging & Profiling & Performance Toolsets
10. Hybrid Programming & Patterns
11. Scientific Visualization & Scalable Infrastructures
12. Terrestrial Systems & Climate
13. Systems Biology & Bioinformatics
14. Molecular Systems & Libraries
15. Computational Fluid Dynamics & Finite Elements
16. Epilogue

+ additional practical lectures & Webinars for our hands-on assignments in context

- Practical Topics
- Theoretical / Conceptual Topics

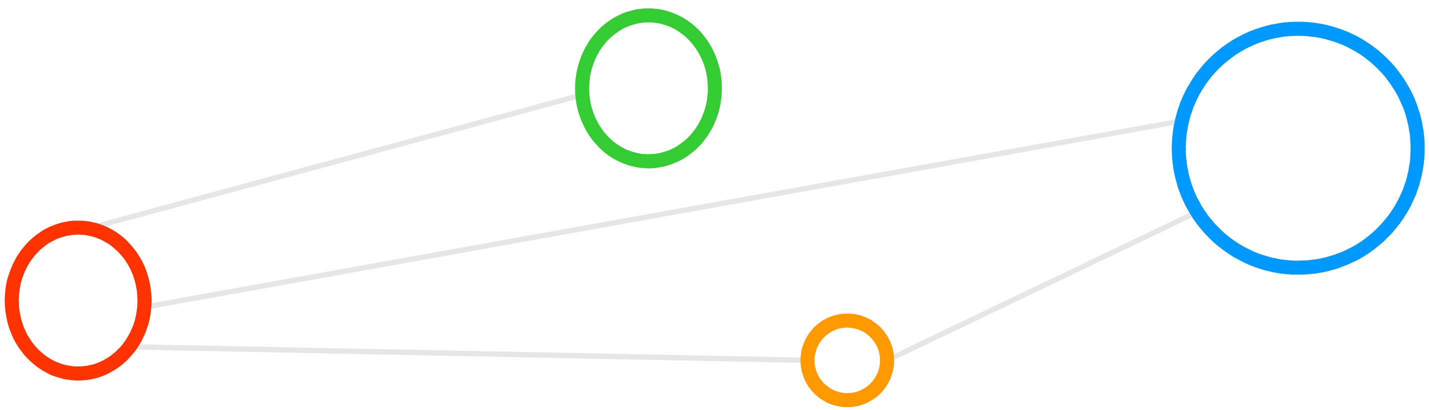
Outline

- Terrestrial Systems
  - Numerical Simulations using known Physical Laws
  - ParFlow Hydrology Model Application Example
  - CLM Land-Surface Model Application Example
  - COSMO Weather Model Application Example
  - Coupling Models via OASIS Coupler & Performance Analysis
- Climate
  - Numerical Weather Prediction (NWP) for Weather Forecasts
  - Role of Partial Differential Equations (PDEs)
  - Weather Research & Forecast (WRF) Model Application
  - WRF Parallel I/O using pNetCDF Parallel File Formats
  - Different Application Areas in Context

- **Promises from previous lecture(s):**
- ***Practical Lecture 0.2:*** **Lecture 12 & Lecture 13 provides more insights about selected applications in Terrestrial Sytems & some applications in Neuroscience**
- ***Lecture 2:*** **Lecture 12 – 15 will offer more insights into a wide variety of physics & engineering applications that take advantage of HPC with MPI**
- ***Lecture 3, 5, 10:*** **Lecture 12 will provide more details on using different domain decompositions for terrestrial systems and climate simulations on HPC**
- ***Lecture 3:*** **Lecture 12 – 15 will provide details on applied parallelization methods within parallel applications & domain/functional decomposition**
- ***Lecture 5:*** **Lecture 12 will provide more details on using blocking vs non-blocking communication in terrestrial systems & HPC climate simulations**
- ***Lecture 10:*** **Lecture 12 will provide more details on how to couple scientific simulation codes that simulate parts of a domain with different physics**

- **Note that this lecture is only a short lecture that usually needs a full course**
- **The goal is to understand selected HPC application fields & provide a few pointers to other advanced related university courses/topics/tutorials**

Terrestrial Systems

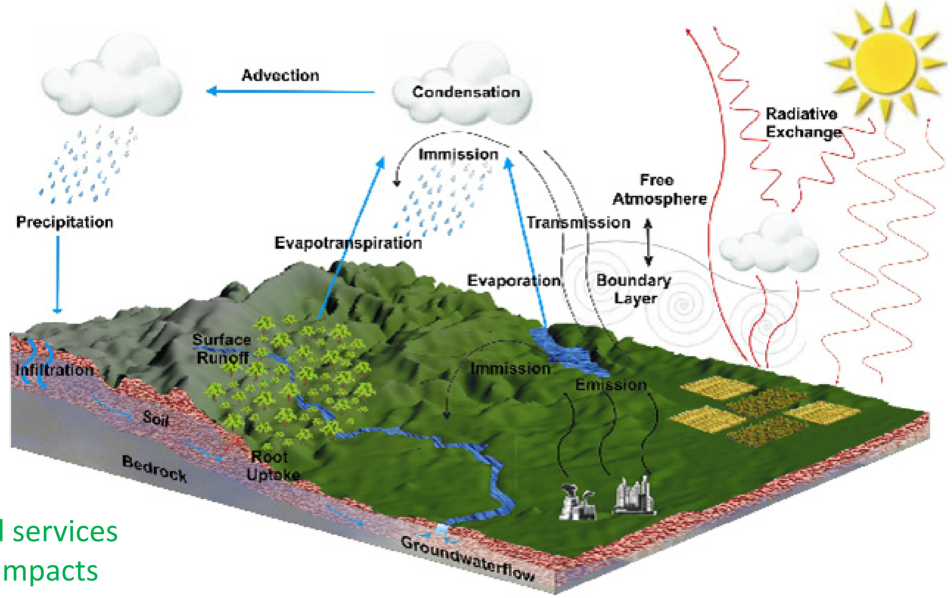


Terrestrial Systems – Motivation

- Selected Motivations
  - Understand global environmental change (e.g. climate) affecting terrestrial systems at all scales
  - Increase understanding of many physical processes on earth (latin terra) that are still poorly understood
  - Work towards better reproducability of models

Physical system changes are accompanied by major state changes of land surfaces & ecosystems

- **Terrestrial systems represent a class of applications that perform numerical HPC simulations of variable complexity of terrestrial systems processes across different scales & regions**



State changes of land surfaces & ecosystems and services provided by them have multiple socioeconomic impacts

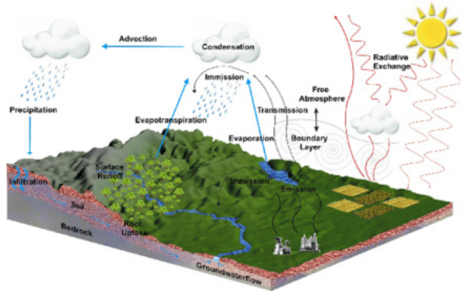
modified from [16] SimLab Terrestrial Systems

Terrestrial Systems – Modelling Dynamical Systems

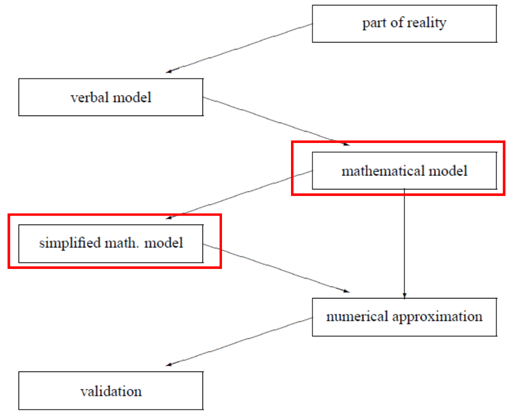
- Evolution in time (and space) is of interest
  - Behavior of a whole ecosystem in time
  - Dynamical systems:
    e.g. economic processes, movement of a fluid, …
  - (cf. simple Jacobi example & heat equation)
- How to model 'evolution' of a system
  - A dynamical system consists of its state (e.g. input data) and a some 'rules'
  - Rules determine how the dynamic system will evolve over time
  - Rules governing the evolution are 'physical laws/equations for different system elements'

[17] Introduction to SC

- **In order to investigate a real system's behaviour by computing, a mathematical model is needed**
- **A dynamical system is some realistic system whose evolution in time is of interest**

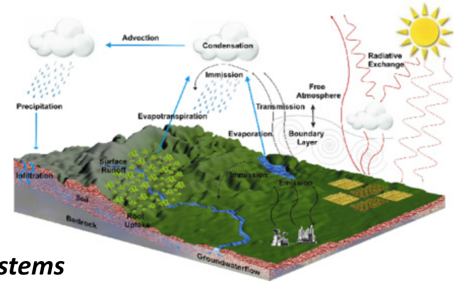


[16] SimLab Terrestrial Systems



Terrestrial Systems Example – Need for Numerical Methods in HPC – Revisited

- Behaviour ‘governed by equations‘ are computed
  - Nature is (too) complex & interconnected: simplification
- Behaviour governed by ‘difference equations‘
  - System state only change at discrete instants of time
  - System state ‘not change in time continously‘
- Behaviour governed by ‘differential equations‘
  - System state evolves ‘continously in time‘
- Selected ‘scientific questions‘ for simulations
  - Under what circumstances will a system evolve into an ‘equilibrium–state’ (state which does not change)
  - Under what circumstances will the system evolve into a ’periodic state’ (states the system return to over time)



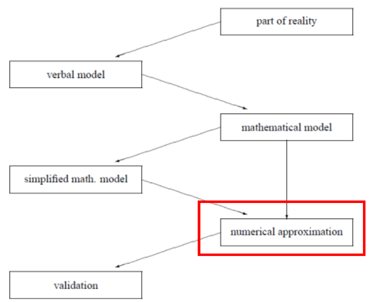
[17] Introduction to SC

[16] SimLab Terrestrial Systems

(solutions can be computed simply by applying definitions iteratively)

- **Solving some mathematical problems & equations is too computational intensive → approximate**
- **Numerical methods are methods that obtain numerical approximation solutions to problems**

(harder to solve, e.g. initial value problem)



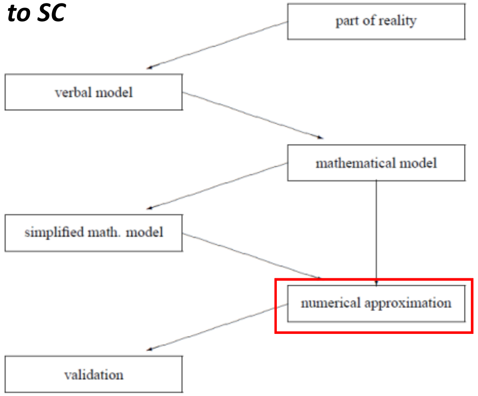
Terrestrial Systems – Role of Partial Differential Equations (PDEs) – Revisited

- HPC simulation modelling
  - PDEs enable rates of change (of continous variables)
  - PDEs used to formulate problems involving functions of several variables
  - PDEs describe a wide variety of phenomena (e.g. sound, heat, electrostatics, fluid flow, etc.)
  - PDEs model multi-dimensional dynamical systems
- Differences to 'ordinary differential equations'
  - Ordinary differential equations deal with functions of a single variable and their derivatives
  - Ordinary differential equations model one-dimensional dynamical system

modified from [18] Wikipedia on 'Partial Differential Equation'

Solving those equations is often too complicated computationally expensive or impossible to analytically compute driving the need for numerical approximation

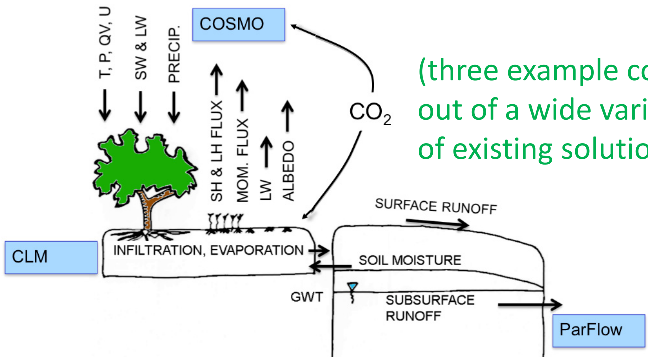
[17] Introduction to SC



- **HPC models often use toolkits (e.g. PETSc) for Partial Differential Equations (PDEs) that are differential equations that contains unknown multivariable functions and their partial derivatives**
- **A general method in HPC modelling use parallel PDEs tools to approximate solutions to problems**

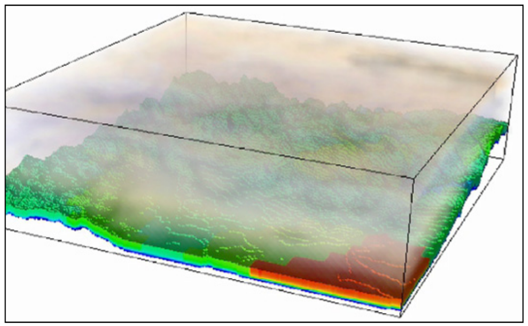
Terrestrial Systems – Numerial HPC Simulations using Multi-Physics

- Numerical models & simulations
  - Investigate multiple terrestrial system processes as a whole
  - Enable sustainable management of terrestrial systems
  - Simulate complex, non-linear transport processes of energy, mass and momentum
  - Create interactions and feedback mechanisms between different compartments of the coupled geo-ecosystem (e.g. subsurface, land-surface, atmosphere, reservoirs, etc.)
  - Varying scales: multiple spatio-temporal scales and high resolutions
  - Potentially long runtimes & use 'ensemble simulations'



(three example codes out of a wide variety of existing solutions)

[16] SimLab Terrestrial Systems

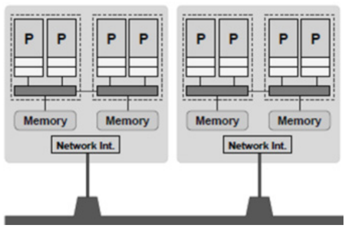


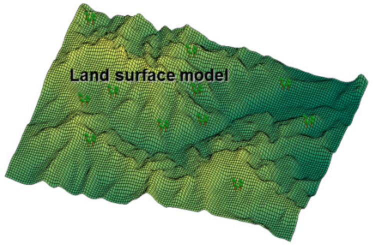
➢ **Lecture 13 provides more details on general & so-called ensemble methods to estimate uncertainties that are often used in HPC**

Towards Realistic Simulations – Reviewing ParFlow, CLM & COSMO Models

- **CLM enables the parallel simulation of land-surface with physical & chemical & biological processes**

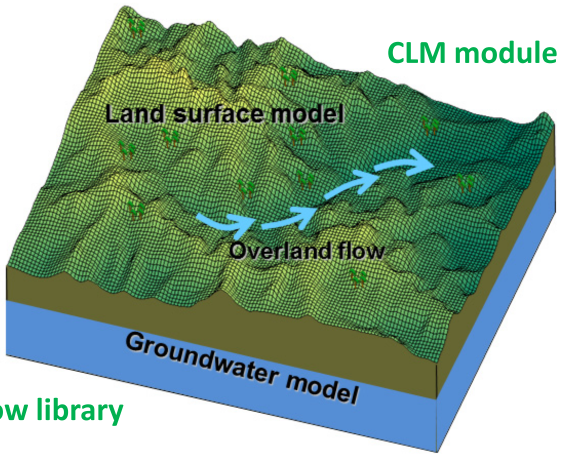
[20] CLM Web page



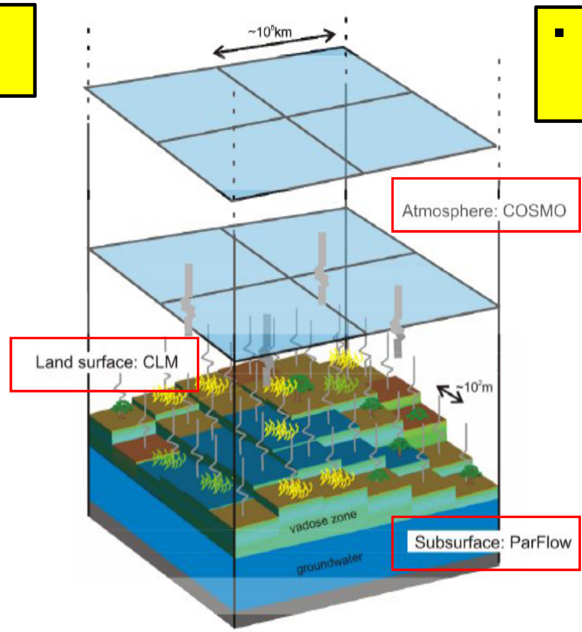


[19] R. Maxwell

CLM module



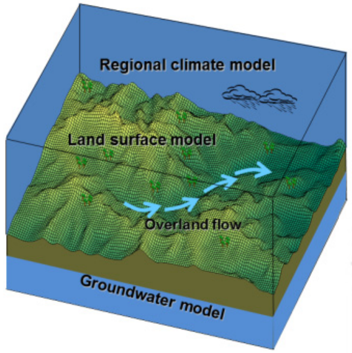
ParFlow library



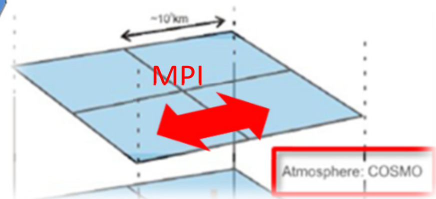
[21] ParFlow Web page

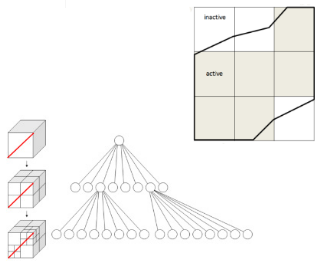
- **ParFlow enables the parallel simulation of hydrology processes with (sub-)surface fluid flows**

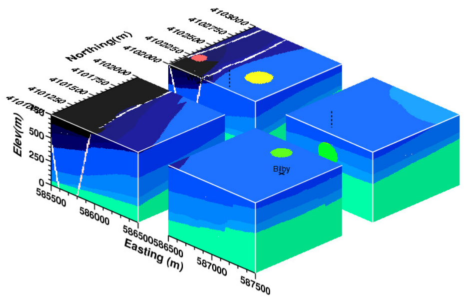
- **COSMO enables the parallel simulation of detailed regional atmospheric model processes**



[22] COSMO Web page

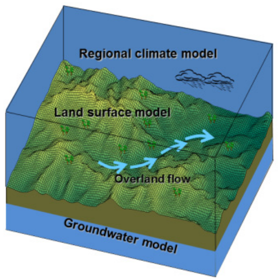


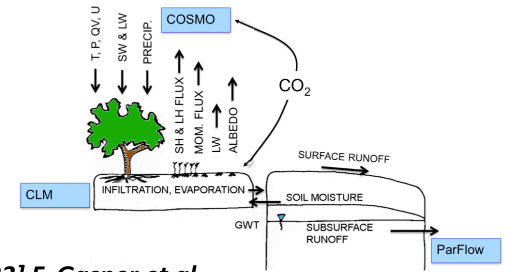




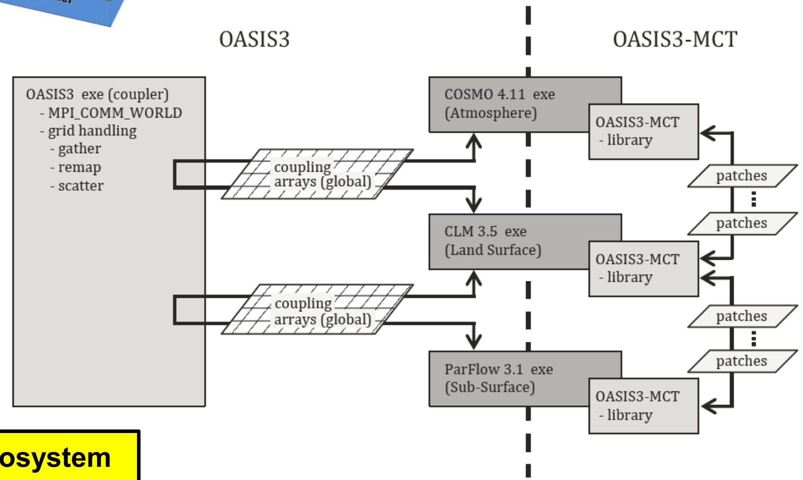
Terrestrial Systems – Coupling Different Parallel Libraries using OASIS Coupler

- Requires a coupling technique running on a HPC machine
  - Example: OASIS3 coupler for ParFlow, CLM & COSMO
  - 1+3 parallel applications together referred to as 'TerrSysMP parallel coupled application'
  - OASIS3 is a separate executable that manages data exchange between others
  - Coupling data arrays are repartitioned to the full domain by OASIS
  - OASIS3-MCT library is part of each component model
  - Coupling arrays only consist of the local fraction of full domain
  - Routed by OASIS to the destination processor





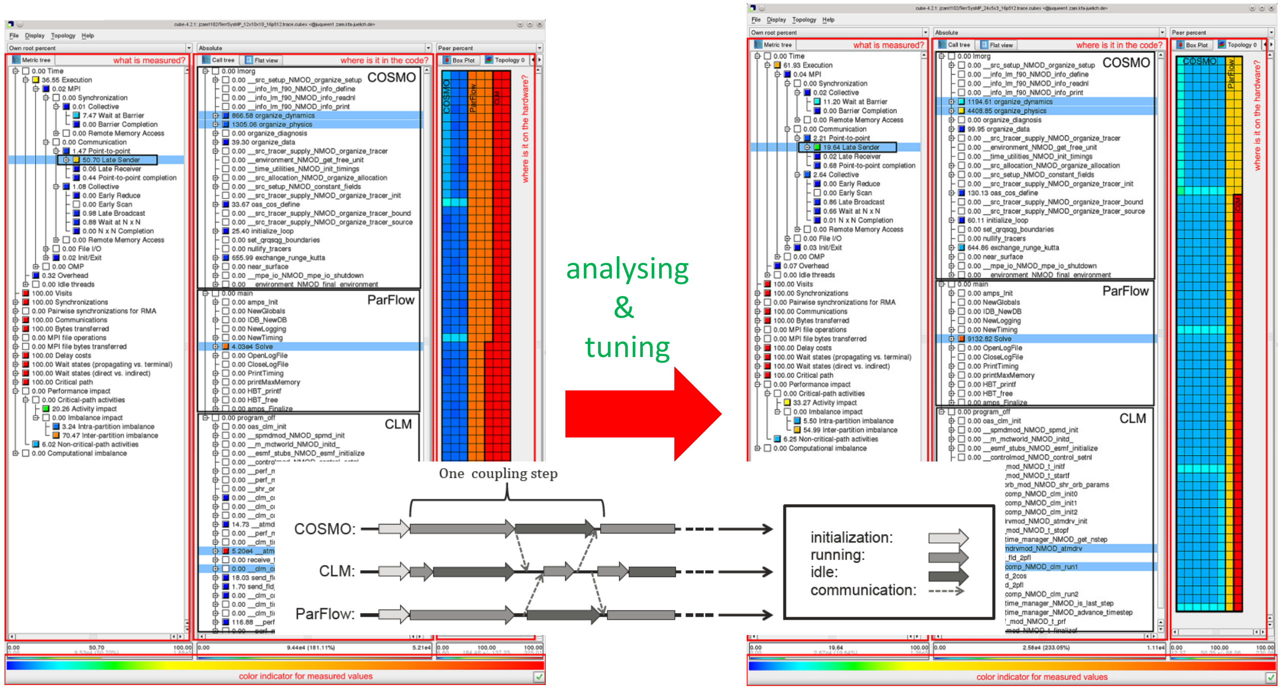
[23] F. Gasper et al.



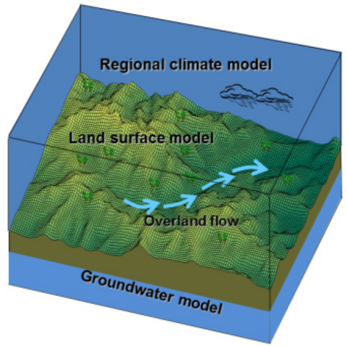
- **Coupled codes execute n different parallel application codes together to simulate one ecosystem**
- **Coupled codes require another separate executable that is a coupler exchanging global data**

Terrestrial Systems – Coupling & Performance Analysis for Fine-Tuning

- Performance optimization required (cf. Lecture 9)
  - Using tool SCALASCA & resources are distributed according to load (better load balance)
  - LateSender wait state is significantly reduced



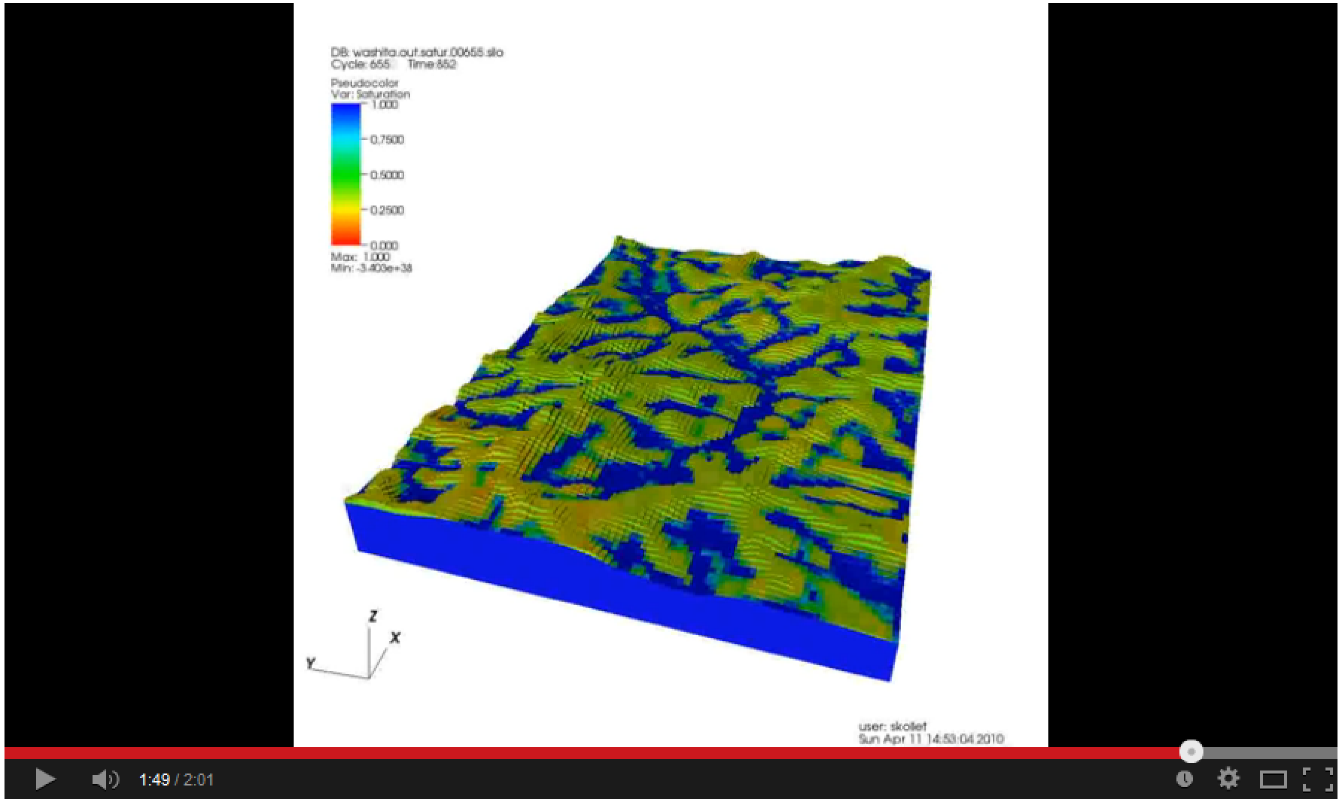
Before:
Processor distribution
192 COSMO
160 ParFlow
160 CLM



After:
Processor distribution
384 COSMO
80 ParFlow
48 CLM

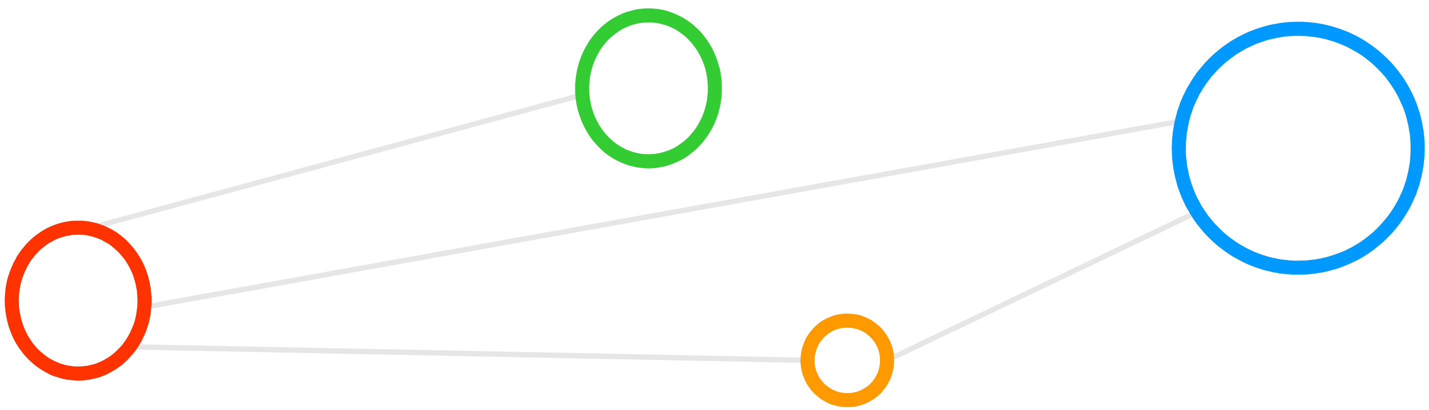
[23] F. Gasper et al.

[Video] Terrestrial Systems with ParFlow coupled with CLM



[5] YouTube Video, ParFlow coupled with CLM

Climate



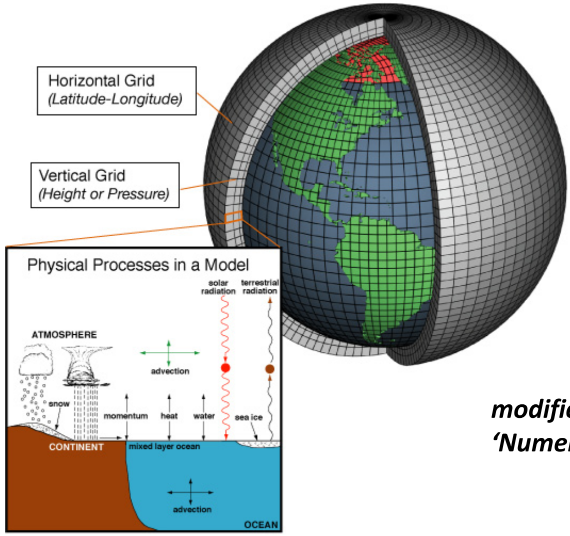
Complex Climate Example – Numerical Weather Prediction (NWP) & Forecast

- Application areas
  - Global & regional short-term weather forecast models in operations
  - Perform long-term climate prediction research (e.g. climate change, polar research, etc.)
- NWP model characteristics
  - Use ordinary/partial differential equations (PDEs) (i.e. use laws of physics, fluids, motion, chemistry)
  - Domain decomposition example: 3D grid cells
  - Computing/cell: winds, heat transfer, solar radiation, relative humidity & surface hydrology
  - Interactions with neighboring cells: used to calculate atmospheric properties over time

▪ Numerical Weather Prediction (NWP) uses mathematical models of the atmosphere and oceans to predict the weather based on current weather observations (e.g. weather satellites) as inputs

▪ Performing complex calculations necessary for NWP requires supercomputers (limit ~6 days) using HPC techniques

▪ NWP belongs to the field of numerical methods that obtain approximate solutions to problems → certain uncertainty remains



modified from [7] Wikipedia on 'Numerical Weather Prediction'

Role of Partial Differential Equations (PDEs) in Atmospheric Research (1)

- HPC Atmospheric Models
  - Simulations produce meterological information for given locations
  - Different ‘temporal resolutions/scales‘: future times, days to decades
  - Different ‘spatial solutions/scales‘: meters to kilometers
  - Use primitive equations to enable model evolution over space and time

- Set of Primitive Equations
  1. Conservation of momentum: Describe hydrodynamical flow on the surface of a sphere (e.g. vertical motion smaller than horizontal motion)
  2. Thermal energy equation: Overall temperature of the modelled system in relation to heat sources and sinks
  3. Continuity equation: Describe the conversation of mass

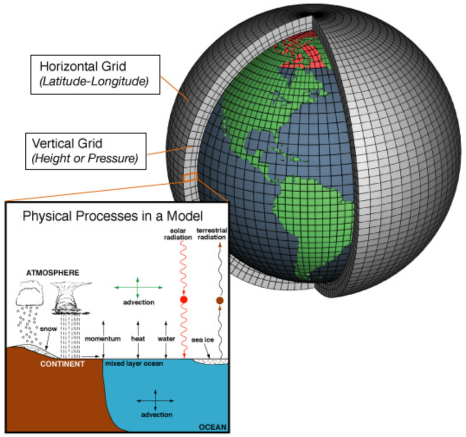
> - **Primitive equations are a set of nonlinear differential equations that are used to approximate global atmospheric flow in atmospheric models and predict/simulate future states of atmospheres**

modified from [8] Wikipedia on ‘Primitive Equations’

Role of Partial Differential Equations (PDEs) in Atmospheric Research (2)

- HPC Model evolution over space and time
  - Based on primitive equations (alongside e.g. gas laws)
  - Simulations shange of density, pressure, potential temperature scalar fields, air velocity (aka wind) vector fields of the atmosphere over time
- Computational challenges
  - Nonlinear PDEs are impossible to solve exactly through analytical methods
  - Idea is to obtain approximate solutions with numerical methods
- Simulation over time
  - Initialization of equations based on analysis data or research question
  - Rates of changes determined via a time increment known as 'time step'
  - Approach is repeated until solution reaches the desired forecast time

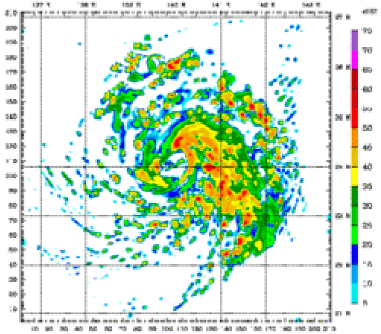
- **Simulations over time need to maintain 'numerical stability': the length of the time step chosen within the model is related to the distance between the points on the computational grid**



modified from [7] Wikipedia on 'Numerical Weather Prediction'

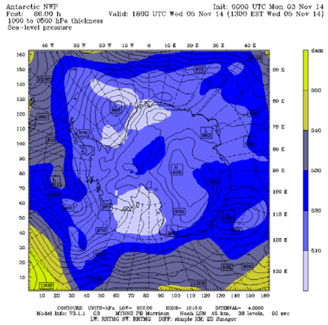
Weather Research & Forecast (WRF) Model Parallel Application – Examples

[9] Wikipedia on 'WRF'



WRF model output showing simulated radar reflectivity (rBZ) for Typhon Mawar (3.3km grid)

[10] Polar WRF

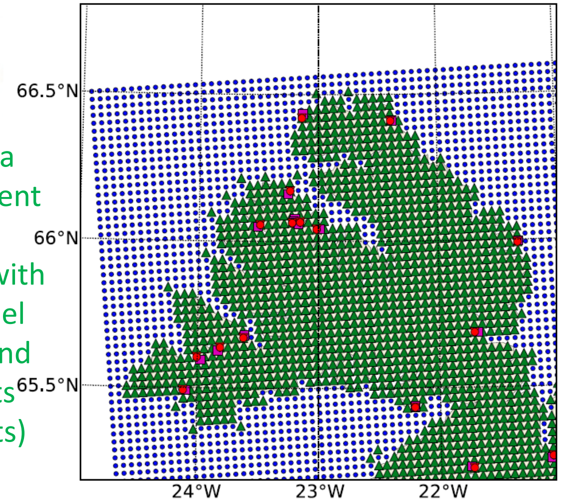


WRF polar model output showing 1000 – 500 hPa thickness & sea level pressure

[11] Evaluation of WRF Mesoscale model

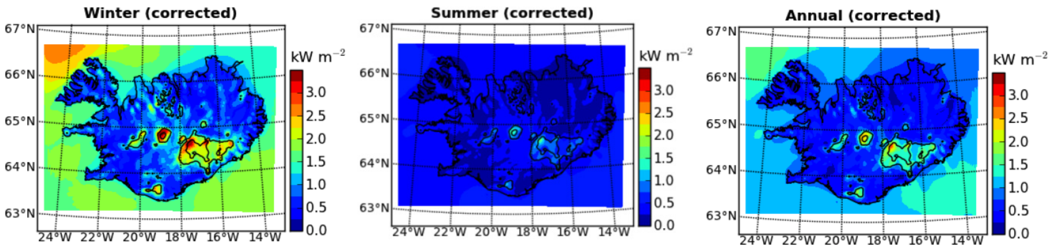
Veðurstofa Íslands

Align data measurement stations in Iceland with WRF model (closest land gridpoints as red dots)



Veðurstofa Íslands

[12] Iceland wind energy potential study, 2013



WRF model output showing wind power density across iceland at 50 mAGL

- **Software package Weather Research and Forecasting (WRF) includes parallelization techniques and enables a wide range of meteorological applications across scales (meters – 1000 of KMs)**

WRF Model Parallel Application – Software

- Weather Research and Forecasting (WRF) model
  - Takes advantage of PDEs (and parallel solvers)
  - Maintained and support as a community model
  - Plug-compatible modules for extensions
  - Research advances have direct path to operations
  - Numerous physics options (link with the broader HPC modeling community) (e.g. air quality modeling)

code used for daily weather forecasts by MetOffices worldwide as service to tax payers

tax payers pay some scientists to better the WRF model
→ ROI / impact over years

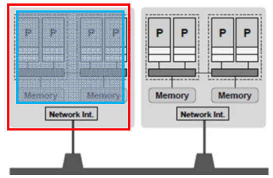
- The WRF model is a NWP system that enables the simulation and prediction of the atmosphere
- It is a scalable parallel HPC simulation for distributed-memory & shared-memory systems

[13] WRF model Webpage

- Selected software package features
  - Available as open-source tool implementing parallelization techniques
  - Implements a modular & hierarchical design
  - Supports a model coupling infrastructure & NetCDF data format support
  - Enables integration into bigger earth system model frameworks

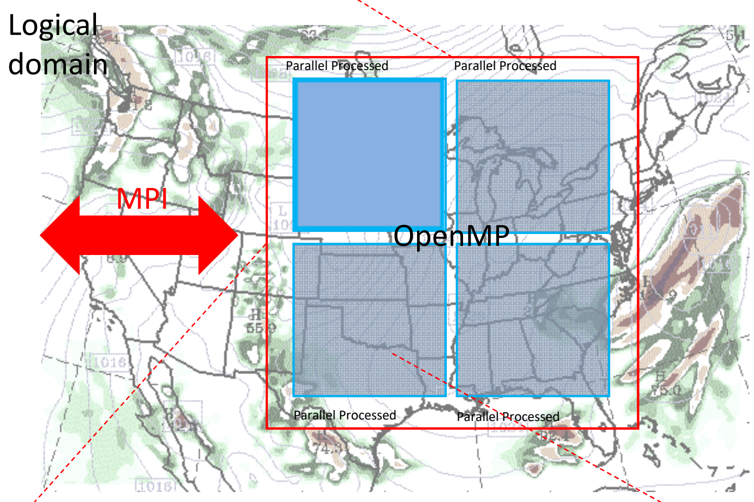
WRF Model Parallel Application – Parallelization Approach (1)

- Parallel simulation sciences
  - E.g. reflecting real data obtained from observations, analyses, etc.
  - E.g. enable idealized atmospheric conditions
- Approach
  - Implements 'hybrid programming' using OpenMP and MPI together (cf. Lecture 10)
  - Use of 'domain decomposition' (cf. Lecture 3) dividing work
  - Model domains are decomposed for parallelism on two-levels using 'patches' and 'tiles'



(patch: section of model domain allocated to a distributed memory node)

(mediation layer solver or physics driver)



(one patch is divided into multiple tiles)

(tile: section of a patch allocated to a shared-memory processor within a node)

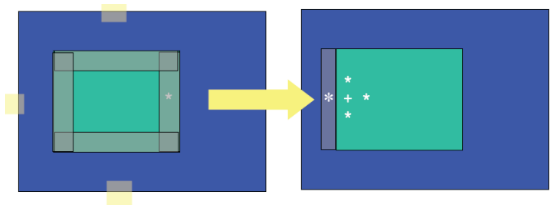
modified from [14] WRF – Code and Parallel Computing

WRF Model Parallel Application – Parallelization Approach (2)

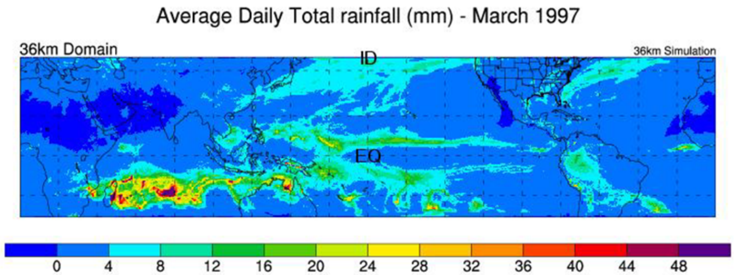
- Usage for ‘halo‘ regions
  - Code example based on Fortran
  - Horizontal data dependencies
  - E.g. i+1, i+1, etc.: indexed operands may lie in the patch of a neighboring processor
  - Problem: neighbor‘s updates to such an element of the array is not accessible on this processor

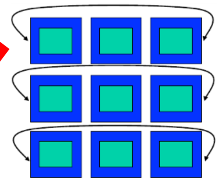
```
                         (module_diffusion.F )

SUBROUTINE horizontal_diffusion_s (tendency, rr, var, . . .
. . .
   DO j = jts,jte
   DO k = kts,ktf
   DO i = its,ite
      mrdx=msft(i,j)*rdx
      mrdy=msft(i,j)*rdy
      tendency(i,k,j)=tendency(i,k,j)-                                  &
           (mrdx*0.5*((rr(i+1,k,j)+rr(i,k,j))*H1(i+1,k,j)-              &
                      (rr(i-1,k,j)+rr(i,k,j))*H1(i  ,k,j))+             &
            mrdy*0.5*((rr(i,k,j+1)+rr(i,k,j))*H2(i,k,j+1)-              &
                      (rr(i,k,j-1)+rr(i,k,j))*H2(i,k,j  ))-             &
            msft(i,j)*(H1avg(i,k+1,j)-H1avg(i,k,j)+                     &
                       H2avg(i,k+1,j)-H2avg(i,k,j)                      &
                                )/dzetaw(k)                              &
           )
   ENDDO
   ENDDO
   ENDDO
. . .
```



(halo updates: get values from memory of left processor to memory of right neighbour processor)



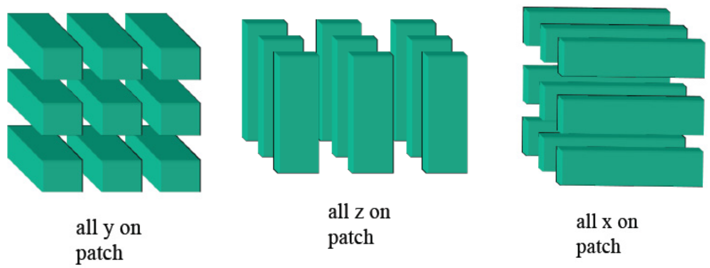


(Periodic boundary updates use interprocess communication)

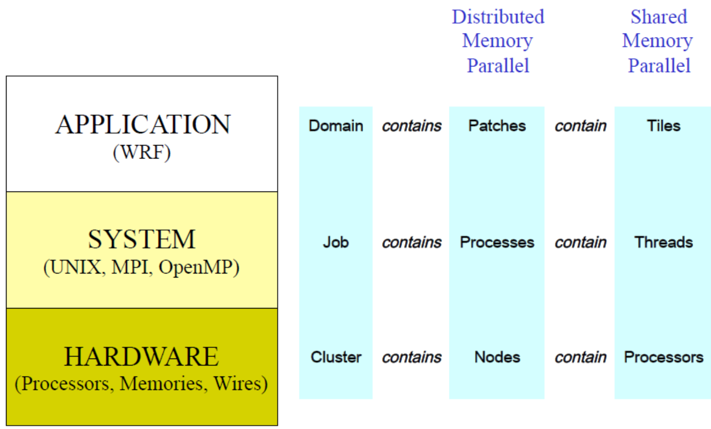
modified from [14] WRF – Code and Parallel Computing

WRF Model Parallel Application – Patches & Terminologies

- Usage for transposes
  - Different parallel transposes are supported
  - Take advantages of MPI



- Overview of parallelization
  - HPC terminology vs. application domain-specific terminology
  - Evolved differently in time

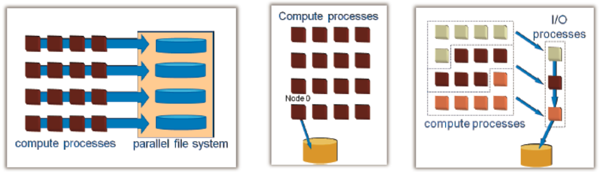


- **One of the most common misunderstandings between the technical HPC community and the application domain-specific communities (e.g. climate) are wrongly interpreted terminologies**

modified from [14] WRF – Code and Parallel Computing

WRF Model Parallel Application – Parallel I/O & Data Types

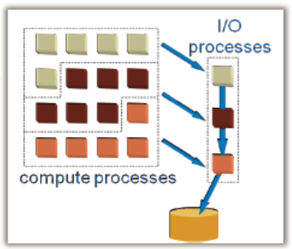
- Need for Parallel I/O
  - WRF is output-bound ('writes costs much')
- Use Serial & parallel NetCDF
  - Provides an I/O layer implemented with parallel NetCDF (pNetCDF)
  - I/O performance gain is considerable against using not pNetCDF

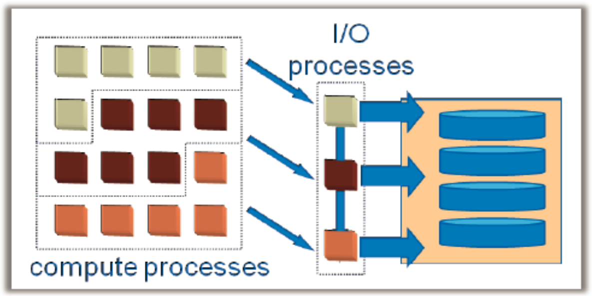


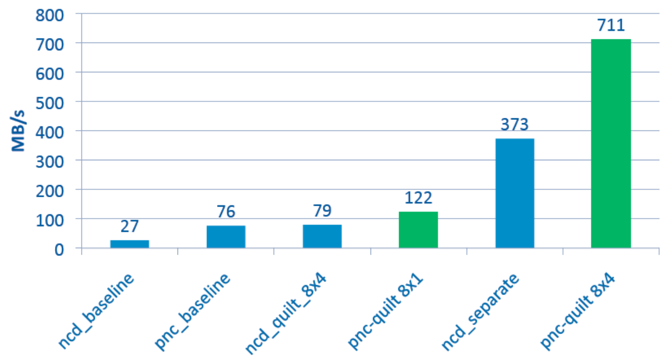
(different options that do not scale)

[15] Opportunities for WRF Model Acceleration

Serial NetCDF collected and written by gangs of MPI tasks (quilting)
Parallel NetCDF written to single files by all MPI tasks in a gang

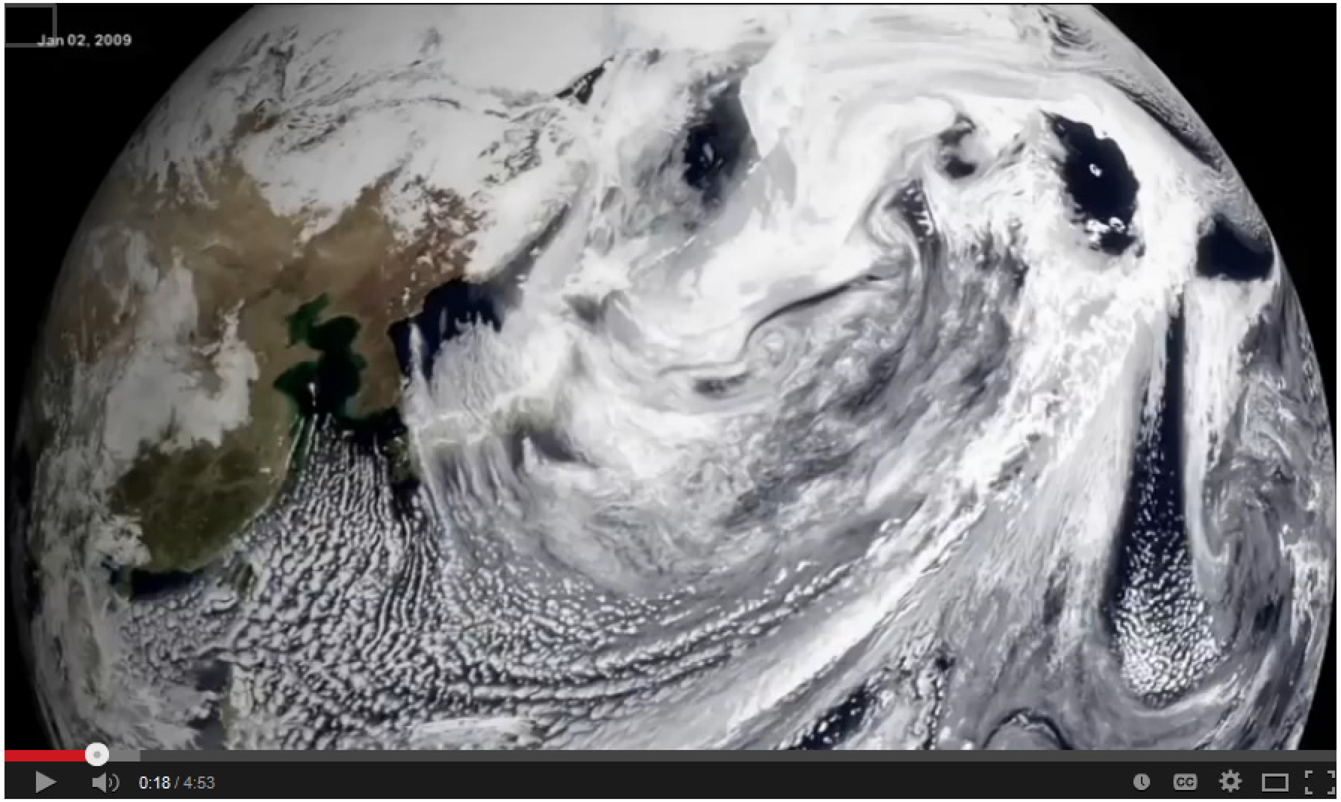






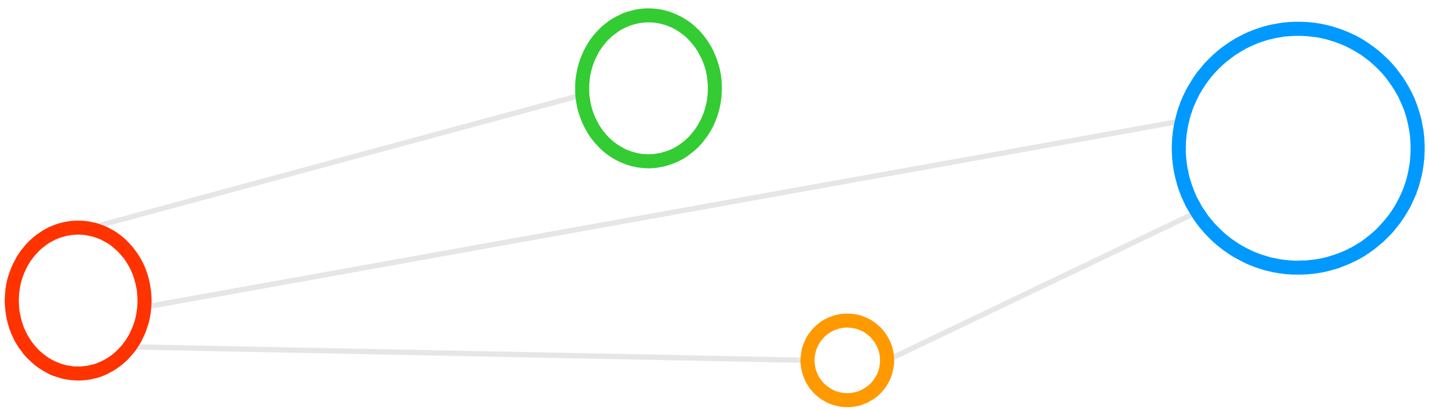
- **Parallel NetCDF can be used to significantly improve I/O output performance of WRF codes**

[Video] Climate Modeling with Supercomputers



[6] YouTube Video, Climate modelling with Supercomputers

Lecture Bibliography



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