High Performance Computing
ADVANCED SCIENTIFIC COMPUTING

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SHORT LECTURE 12

Terrestrial Systems and Climate

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Webinar
Review of Short Lecture 11 – Scientific Visualization & Scalable Infrastructures

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)

[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

[4] PRACE RI

- 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

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**High Performance Computing**
(a field of constant changes)

**HPC Course**

Domain-specific Science & Engineering A

Domain-specific Science & Engineering B

Domain-specific Science & Engineering C

Domain-specific Science & Engineering D
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
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 Systems & 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 – 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

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

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

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 some ‘rules’
  - Rules determine how the dynamic system will evolve over time
  - Rules governing the evolution are ‘physical laws/equations for different system elements’

[16] SimLab Terrestrial Systems

[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
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 continuously’
- 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 )

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Solving some mathematical problems & equations is too computational intensive \( \rightarrow \) approximate

Numerical methods are methods that obtain numerical approximation solutions to problems
Terrestrial Systems – Role of Partial Differential Equations (PDEs) – Revisited

- HPC simulation modelling
  - PDEs enable *rates of change* (of continuous 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*

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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 contain unknown multivariable functions and their partial derivatives*

*A general method in HPC modelling use parallel PDEs tools to approximate solutions to problems*
Terrestrial Systems – Numerical 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’

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

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

[21] ParFlow Web page

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

[22] COSMO Web page

R. Maxwell

- CLM Web page

- ParFlow Web page

- COSMO Web page

Short Lecture 12 – Terrestrial Systems and Climate
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

- 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**
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

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

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

- **HPC Atmospheric Models**
  - Simulations produce meteorological 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

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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 change 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

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


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


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

[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)
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)

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

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
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
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’

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

(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

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

Short Lecture 12 – Terrestrial Systems and Climate
[Video] Climate Modeling with Supercomputers

[6] YouTube Video, Climate modelling with Supercomputers
Lecture Bibliography
Lecture Bibliography (1)

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- [20] Community Land Model (CLM), Online: http://www.cgd.ucar.edu/tss/clm/
- [22] Consortium for Small-scale Modeling (COSMO), Online: http://www.cosmo-model.org/