Parallel programming with MPI in a computer cluster

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Parallel programming

- Serial computing
  - Single process unit ("core") used for solving a problem
- Parallel computing
  - Problem is split into smaller subtasks
  - Processed simultaneously using multiple cores

MPI

- Message Passing Interface.
- Standardized and portable message-passing system designed to function on a wide variety of parallel computers.
- Leading standard for message-passing libraries for parallel computers.
- Application programming interface (API) for communication between separate processes.
- Allow users to write portable programs in Fortran, C, or C++.
- For more detailed MPI tutorial see e.g. the parallel programming materials in `https://www.csc.fi/web/training/materials`.

MPI with python

- mpi4py
- A package enabling applications to exploit multiple processors using standard MPI “look and feel” in Python scripts
- The interface was designed with focus in translating MPI syntax and semantics of standard MPI-2 bindings for C++ to Python
- Built-in parallel computation options also in other packages, e.g. in emcee (affine invariant sampling):
  `http://dfm.io/emcee/current/user/advanced/`

Computational resources

- tuorla42
- titan.utu.fi
- Use ssh to contact

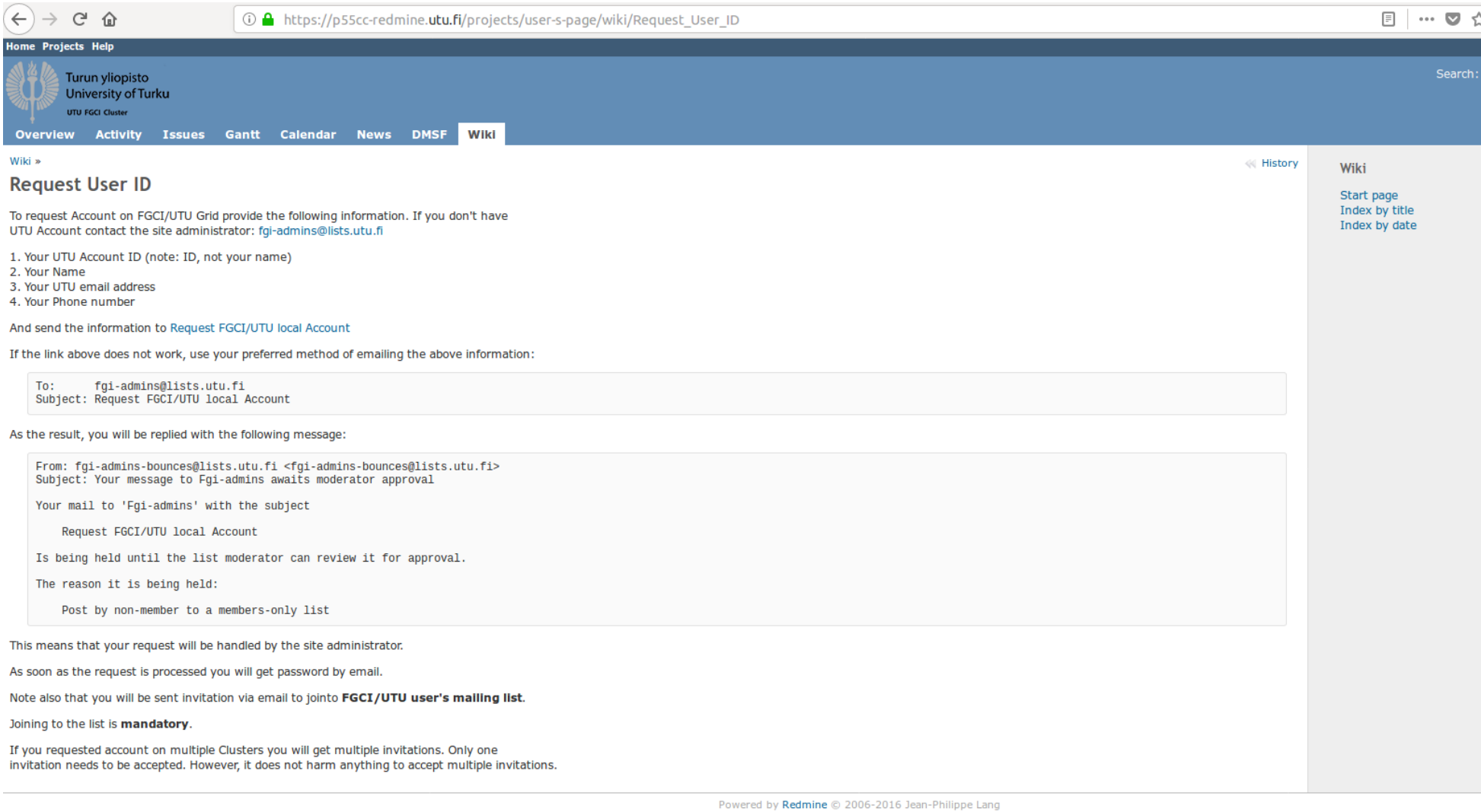
Tuorla42

- The server will be upgraded soonish (access in the future through containers)
- CPU(s): 48
- On-line CPU(s) list: 0-47
- Thread(s) per core: 2
- Core(s) per socket: 12
- Socket(s): 2

Titan

- A computer cluster
- Located at Turku but part of Finnish Grid and Cloud Infrastructure (FGCI)
- 260 cores (10 nodes + 1 largemem node)

Titan


https://p55cc-redmine.utu.fi/projects/user-s-page/wiki/Request_User_ID
Home Projects Help
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University of Turku
UTU FGCI Cluster
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Request User ID
To request Account on FGCI/UTU Grid provide the following information. If you don't have UTU Account contact the site administrator: fgi-admins@lists.utu.fi
1. Your UTU Account ID (note: ID, not your name)
2. Your Name
3. Your UTU email address
4. Your Phone number
And send the information to Request FGCI/UTU local Account
If the link above does not work, use your preferred method of emailing the above information:
To: fgi-admins@lists.utu.fi
Subject: Request FGCI/UTU local Account
As the result, you will be replied with the following message:
From: fgi-admins-bounces@lists.utu.fi <fgi-admins-bounces@lists.utu.fi>
Subject: Your message to Fgi-admins awaits moderator approval
Your mail to 'Fgi-admins' with the subject
Request FGCI/UTU local Account
Is being held until the list moderator can review it for approval.
The reason it is being held:
Post by non-member to a members-only list
This means that your request will be handled by the site administrator.
As soon as the request is processed you will get password by email.
Note also that you will be sent invitation via email to jointo FGCI/UTU user's mailing list.
Joining to the list is mandatory.
If you requested account on multiple Clusters you will get multiple invitations. Only one invitation needs to be accepted. However, it does not harm anything to accept multiple invitations.
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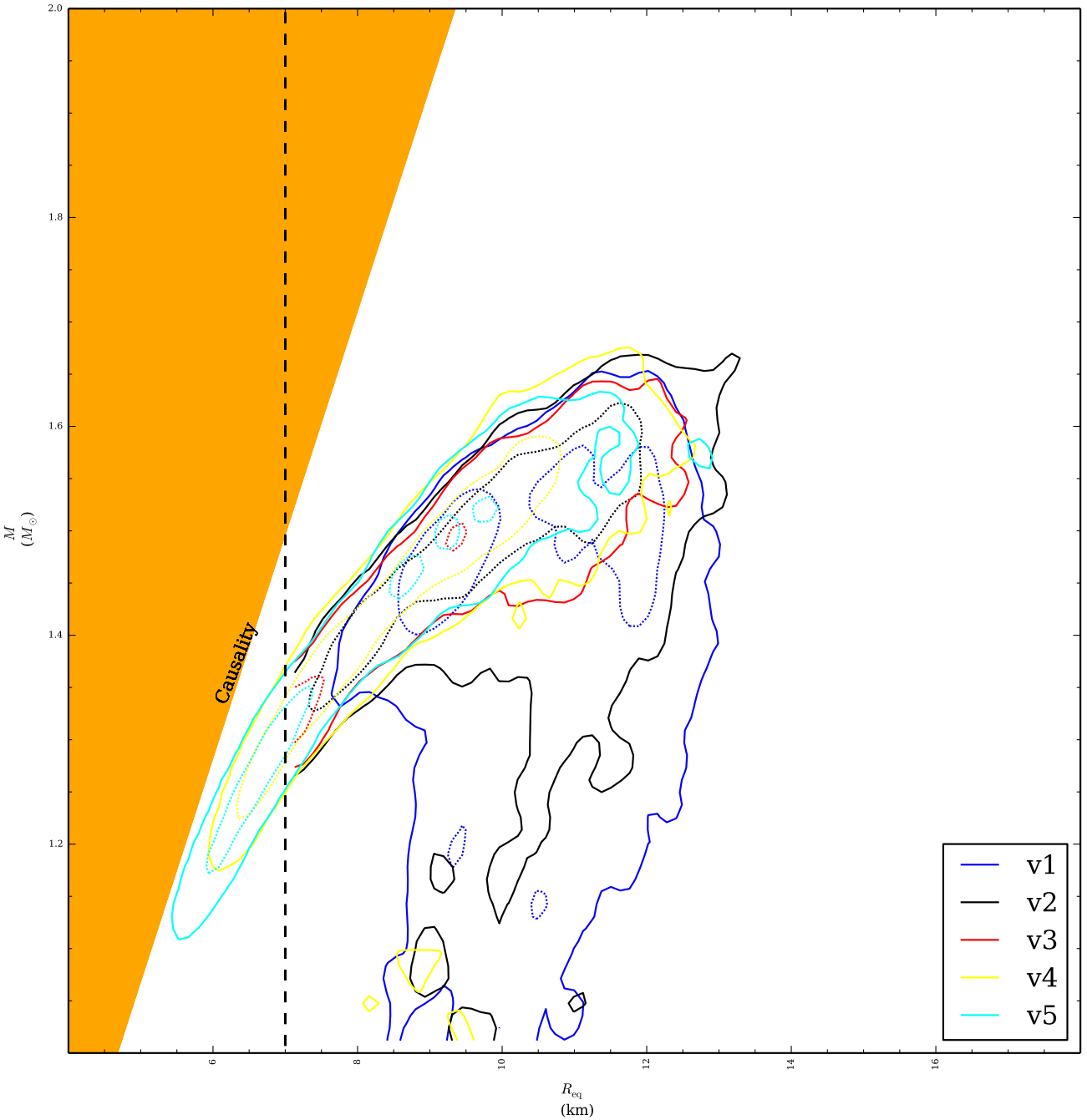
Practical examples

- Introductory excercises for mpi4py: `https://github.com/jbornschein/mpi4py-examples`
- Running the examples in titan.utu.fi (in installation node and how to put in grid usage)
- SLURM-commands: e.g. sbatch, scancel and squeue.

Benefits of parallel computing with Bayesian methods

- You can try to reproduce same distribution calculated independently (but simultaneously) with several cores.
- Slow convergence might still be an issue.
- My experiences: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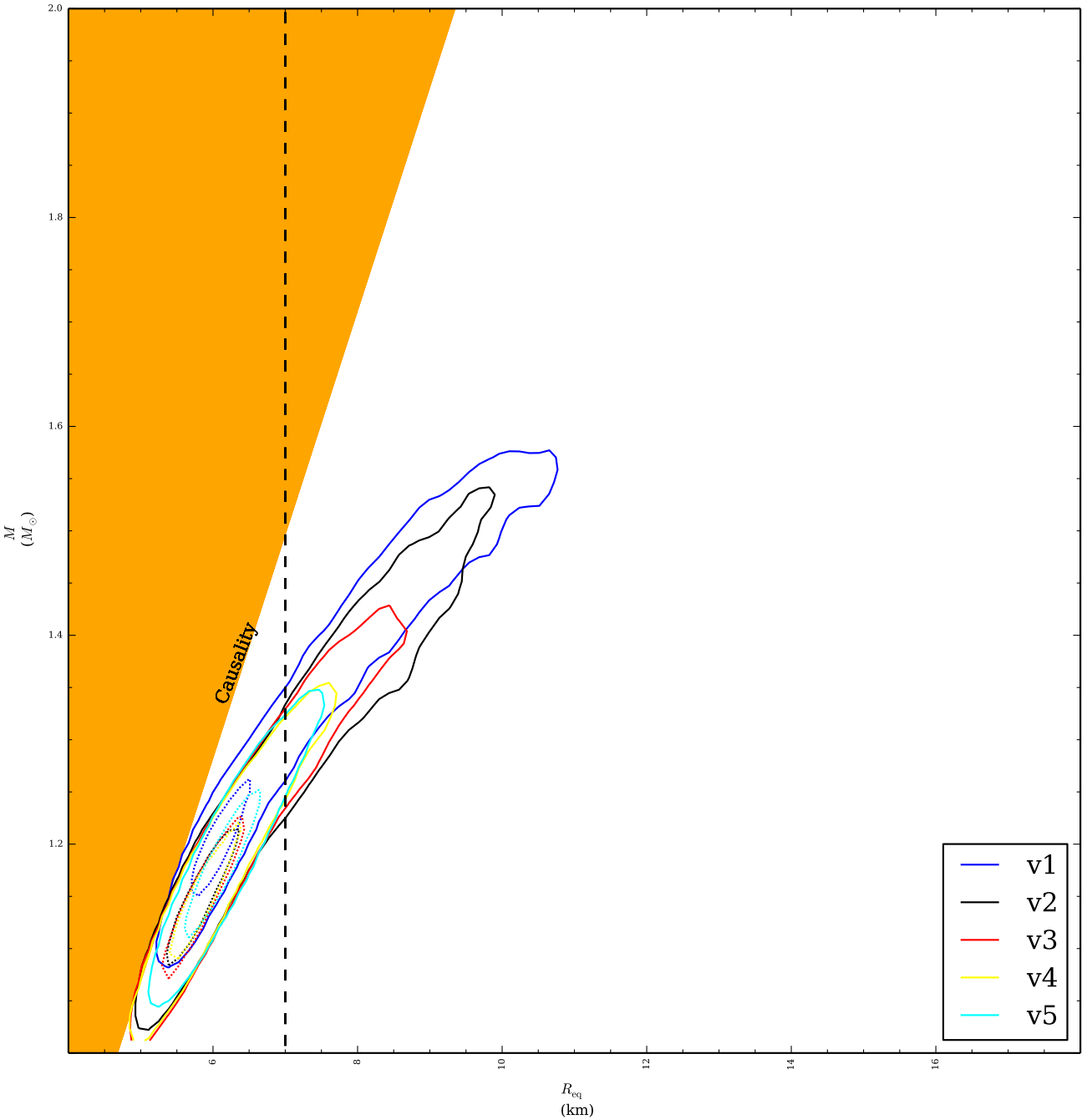
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The End