NLAFET

Parallel Numerical Linear Algebra for Future Extreme-Scale Systems

H2020-FETHPC-2014: GA 671633

D7.2
Collaborative Infrastructure

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1. Executive summary

This document describes the collaborative infrastructure with focus on the NLAFET public website and the internal website consisting of a Wiki and a Forum. In addition, the document outlines how the internal and public source code repositories of the NLAFET library will be set up, as well as the ongoing development of coding styles and developer guidelines for the numerical linear algebra software routines in the NLAFET library. This work is done within WP7 - Dissemination and community outreach.

NLAFET is the acronym for the complete Horizon 2020 FETHPC project title “Parallel Numerical Linear Algebra for Future Extreme Scale Systems” and is used throughout this document.

2. Public website

The NLAFET website is the main dissemination channel for promotion of the project and will function as the public interface of NLAFET. Hence, it contains basic information about the project, the partners involved, how to contact the coordinator, the main focus of the research, and the publication results of the project thus far.

The website is available at www.nlafet.eu and has six main sections:

- **HOME**
  The home page highlights the latest news and a calendar of events. It also contains the login to the internal wiki of NLAFET.
- **ABOUT**
  At top level, this page contains an overview of the background and main aims of the NLAFET project. It also contains coordinator contact information and a list of partners in the consortium (Umeå University, the University of Manchester, INRIA and STFC). In addition, the people involved in the project are presented. Finally, the funding source, the European Commission, is acknowledged, and a link to the projects funded in the FETHPC-2014 call is given.
- **RESEARCH**
  The research to be conducted within NLAFET is structured in four work packages:
  - WP2 – Dense linear systems and eigenvalue problem solvers
  - WP3 – Direct solution of sparse linear systems
  - WP4 – Communication-optimal algorithms for iterative methods
  - WP6 – Cross-cutting issues

  The focus of WP2, WP3, and WP4 is research into extreme-scale parallel algorithms. The focus of WP6 is research into methods for solving important common cross-cutting issues. The work packages are briefly described under designated links. The descriptions will be made richer as the project progresses and new advances and research results are ready to report.

- **USE CASES / APPLICATIONS**
  The algorithms and software developed in the NLAFET project will be evaluated in four complementary real world application domains: materials science, power systems, study of energy solutions, and data analysis in astrophysics. This page contains brief descriptions of these use cases and applications. Information about the results of the validation efforts will be added as soon as they become available. This work will be performed in workpackage WP5 – Challenging applications – a selection.
- **PUBLICATIONS**
  All publications relating to the NLAFET project will be published. The menus include a list of completed public deliverables, list of scientific publications obtained as a result of this project, presentations made in association with this project, and a collection of technical reports (NLAFET Working Notes) emanating from the work.
- **NEWS**
  A range of news items will be presented here. NLAFET news will be updated as the project progresses.

Below, we display a screenshot of the main page of the NLAFET public website. The top banner shows the northern lights above part of the Umeå University campus. The NLAFET headquarters is situated in the MIT (Mathematics and Information Technology) building which is visible below the three first letters of NLAFET.

3. Internal website

Collaboration in the project will be coordinated mainly through the internal website. The internal site is only available to the partners and consists of two components:

- A **wiki** (https://wikis.cs.umu.se/nlafet) that collects currently available information. For example, the state of work in each deliverable, the formal documents and templates, the administrative procedures, etc.
- A **forum** (http://www.nlafet.eu/phpbb/index.php) that enables organized topical discussions within and between partners. There is a separate forum for each deliverable, one for general technical discussions, one for general non-technical discussions, etc.

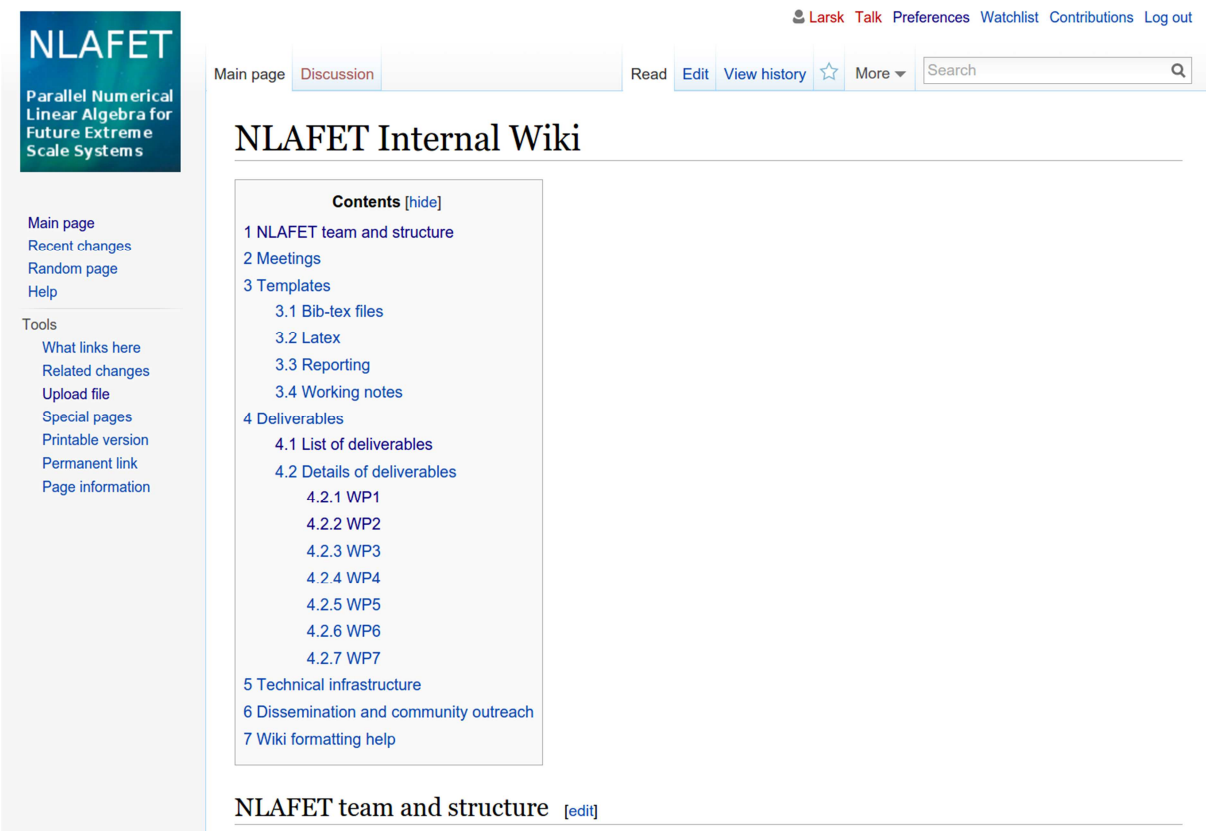
The purpose of the internal website is to enable *transparency*, spontaneous *collaboration*, and a *historical record* of our lines of reasoning. Transparency helps to manage the project by keeping track of work and progress with respect to the various deliverables and to ensure that partners agree on key decisions early in the process. Transparency also encourages spontaneous collaboration to take place. By understanding what is going on in another part of the project, a team member has the opportunity to join the discussion through the forum.

By examining relevant historical threads, new team members can get easy access to the previous discussions and so can participate more quickly and be much more productive.

3.1. Wiki

The NLAFET Internal Wiki contains information of a more permanent character. For example, it lists all pertinent information about the team and its organizational structure. It has a list of previous and upcoming meetings with agendas and minutes. There is a list of templates for deliverables, financial reporting, etc. Most importantly, there is a list of deliverables and a separate page for each deliverable in the project. Each such page documents the team members working on that deliverable, the original formulation in the grant, our current interpretation and elaboration of that specification, as well as our current perception of the best path towards the final target. Finally, a list of current open questions is spelled out to elicit spontaneous collaboration.

Below, a screenshot of the main page of the NLAFET Internal Wiki is displayed.

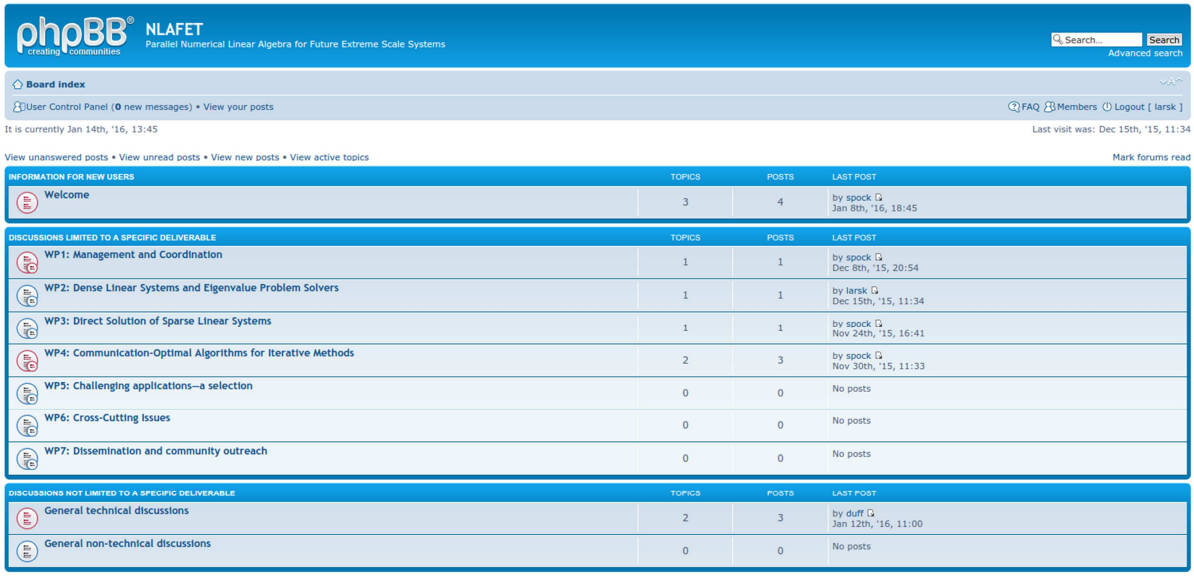


In addition, a screenshot of the Wiki page for deliverable D2.5 Eigenvalue Problem Solvers is displayed below.

3.2. Forum

The forum contains active threads of discussion as well as a complete historical record of previous discussions. The topics reflect the structure of the NLAFET project. The main subdivision is by work package with a separate subforum for each deliverable. There are also subforums for technical and non-technical discussions which are not limited to a specific deliverable. The overall goal is to make the ongoing work transparent and structured. In addition, old threads function as a historical record of previous discussions, particularly useful for new team members. The forum is more structured and searchable than an email inbox will ever be. In addition, team members will get automatic notifications when replies are posted to threads which they are following.

Below, a screenshot of the main page of the NLAFET Internal Forum is displayed.



4. Source code repository

A repository has been created on the CCPForge repository to enable the use of modern software engineering tools for version control, issue tracking, and continuous integration. The main website for this repository is:

http://ccpforge.cse.rl.ac.uk/gf/project/nlafet/

The repository provides a location for the official git repository. Git is a distributed version control tool that allows the creation of local repositories at each of the sites and for individual developers. These local repositories can allow rapid iteration within subteams and git provides an easy mechanism to merge these changes back to the official repository when they are ready. It is also possible to clone the repository using the command:

git clone ssh://anonymous@ccpforge.cse.rl.ac.uk/gitroot/nlafet

Two issue (bug) trackers have been created on the repository: one for internal use by the partners (e.g., tracking features and deliverables), and one for external users to submit bug reports and feature requests.

Continuous Integration has also been enabled. This allows the easy automation of the build process using the Jenkins CI system. Each time a commit is made, it can be configured to build the code and run tests on a range of architectures and under a variety of compilation flags and options to highlight test failures and code regressions as soon as they occur.
A guide will be prepared to accompany the coding guidelines on the best way to utilise these systems to work in a collaborative fashion.

5. Coding styles and developer guidelines

The NLAFET coding styles and developer guidelines are under development. The result will be a living document to be expanded and modified as needed. The purpose is to obtain a clean and consistent codebase that is well-documented, portable and maintainable in the long term. To some extent, the coding styles and guidelines will also adhere to existing software and libraries that are expected to be important several years ahead.

To meet the demands of extreme-scale (and future exascale) systems, the rules and guidelines must take many realities and new developments into account. In addition to program languages (Fortran, C, C++ etc), these include parallel programming and execution models and environments.

Since extreme-scale systems are hierarchical and heterogeneous in nature, we must adopt hybrid models. Today, there are no final standards but features in MPI libraries and OpenMP are evolving to provide reliable extreme-scale programming environments for C++, C, and Fortran, that promise to be portable and sustainable. For example, the OpenMP4.0 standard addresses tasking requirements including Direct Acyclic Graph (DAG) scheduling constructs, and will be complemented by the OpenACC to address accelerators.

In general, the situation is more complicated for distributed memory computing, and the de-facto standards available are based on MPI. New MPI features proposed include asynchronous global and neighbourhood collectives enabling implementation of latency hiding algorithms, and MPI shared memory features enabling use of shared memory between ranks, and thread-like shared memory programming. For distributed memory, we will adopt the PaRSEC scheduler that represents a DAG using a multi-level parameterized task graph (PTG). The PaRSEC project is ongoing research and development. The current version(2.0.0) takes care of inter-node messaging, intra-node multithreading and offloading work to multiple accelerators.