## Imperial College London

## Nektar++ Community and Development Strategy

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Nektar++ Workshop Imperial College London 7th June 2016

## **Overview**

- Nektar++ Community and Support
  - What's new?
  - Accessibility
  - Education
  - Support
- · Improving code stability
  - Developer practices
  - Release schedule
  - Review process
- Summary and What's next?

## Nektar++ Community and Support

The mission of Nektar++ is to make spectral/hp element methods accessible to a broader audience and remove the implementation complexity barrier which limits adoption of these methods.

We are keen to engage with the community of users in their use of Nektar++.



Accessibility (support for range of OSs, packages)



Education (tutorials, documentation)



## What's New?

- Tutorials for new users (more later)
- Redevelopment of Nektar++ website to be more community driven
- User guide available online in HTML form
- · Binary packages now available for a broader range of platforms
- Tested on a wider and more up-to-date range of operating systems



- Now used on a range of supercomputers:
  - SGI ICE (CX2, Imperial College London)
  - Blue Gene/Q (Mira, Argonne National Laboratory)
  - Cray XC30 (ARCHER, UK National Supercomputer)
  - Cray XE6 (Copper, DoD)

#### How can one get Nektar++?



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- Homebrew and MacPorts (OSX):
  - See http://www.nektar.info/ installing-nektar-on-os-x-through-macports-or-homebrew/

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- Source code bundles (self-compile) from http://www.nektar.info
  - Different archive formats (.tar.gz, .tar.bz2, .tar.xz, .zip)
  - Regular releases, but not most recent updates
  - Build against Nektar++ libraries, but no direct means to contribute

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- Git repository
  - Anonymous checkout
    - git clone http://gitlab.nektar.info/clone/nektar/nektar.git
  - Authenticated checkout git clone git@gitlab.nektar.info:nektar/nektar.git

- · Intended to help new users quickly get started with Nektar++
- Low barrier to entry
- Introduce various aspects of the code
  - Basic usage of the solvers
  - Use of the code for specific applications
  - Using the libraries to support writing new code

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  - Using the libraries to support writing new code
- Available both as PDF documents and HTML webpages

http://www.nektar.info/community/tutorials/

Current tutorial selection



• We welcome suggestions for new tutorials!

Each tutorial provides a structured introduction to a topic:

Introduction and goals

Goals

After completing this tutorial, you should be familiar with:

• The concept of Gaussian integration using classical Gauss and Gauss-Lobatto rules in a standard interval  $\mathcal{E} \in [-1, 1]$ .

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#### Context

the use of numerical integration or *quadrature*. The fundamental building block is the approximation of the integral by a finite summation of the form

$$\int_{-1}^{1} u(\xi) d\xi \approx \sum_{i=0}^{q-1} w_i u(\xi_i),$$

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#### Step-by-step tasks, often with partially completed files



#### Task 3.3

Evaluate the previous integral for a quadrature order of  $Q = Q_{\max}$  where  $Q_{\max} = 7$  and 8 to verify that to exactly integrate with Gauss-Lobatto type integration you require an additional quadrature point and weights.

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- · Summary of what has been learnt
- Set of complete solutions

• Versioned with code



Nektar++: Spectral/hp Element Framework

Version 4.4.0

#### User Guide

May 31, 2016

Department of Aeronautics, Imperial College London, UK Scientific Computing and Imaging Institute, University of Utah, USA

- Versioned with code
- User guide



- Versioned with code
- User guide
  - Installation



- Versioned with code
- User guide
  - Installation
  - Solver and Utility usage
  - Examples
  - Input file reference
  - FAQs



Nettar+ is an open source software library currently being developed and designed to provide a toolbox of data structures and algorithms which implement the spectral/hp element method. Netkar+ is the continuation and adaptation of the Netkar flow solver. As opposed to its predecessor which focused on solving fluid dynamics problems. Netkar+ is implemented as a C++ object-oriented toolist which allows developers to implement spectral element solvers for a variety of different engineering problems.

The structure of the Nektar++ library, a collection of different sublibraries, is based upon the typical structure of a global spectral/hp approximation, which is characterized by:

The elemental decomposition of the problem

As for all finite element methods, the computational domain is partitioned into a mesh of many small subdomains or elements. Analogously, the spectral/hp solution is expanded into a series of local expansions, each with support on a single element. This elemental representation enables the treatment of operations on a local elemental basis rather than on global level. This not only simplifies the formulation but also allows many operations to be performed more efficiently.

The introduction of a standard region

The introduction of a standard region allows the expansion basis to be defined just once, that is only on the standard region. All other elements then can be considered as the image of the standard element under a parametric mapping. Consequently, the elemental operations of integration and differentiation can all be executed on the standard element, subject to a proper treatment of the transformation from local (world space) to standard (reference space) coordinates. For curved-sided elements, the mapping from standard element to local element is generally done using an *iso-parametric representation*. In this case, the local geometry is represented with an expansion of the same form and polynomial order as the unknown variables.

This structure, supplemented with building blocks such as block matrix linear algebra routines and automatic data coordinating objects, can be encapsulated in an efficient object-oriented C++ implementation.

This conceptual approach of the software leads to a high user-flexibility, including the selection of the preferred expansion basis, its polynomial order and the preferred numerical quadrature.

The website of the Nektar++ project can be found on: http://www.nektar.info

- Versioned with code
- User guide
  - Installation
  - Solver and Utility usage
  - Examples
  - Input file reference
  - FAQs
- Code documentation
  - Doxygen
  - Detailed implementation specifics

### **Support**

We are striving to build a community around Nektar++

- · Support new users
- Make it easier for users to contribute back to the project.

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- Nektar++ Workshops (now an annual event!)
- Publication list
  - Help us demonstrate the impact of Nektar++
  - We can promote your research

# Nektar++ is a large project and therefore requires careful management of code changes to maintain stability.

We have implemented a range of tools and best practices to help facilitate this.

In the past year, there have been three key changes:

- Code review process
- · Release model
- Change log and contribution guide

These build on a range of development practices we have already implemented.

What development practices support a large multi-plaform collaborative software project such as Nektar++?

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Version-control (Git + GitLab)

#### Issue tracking (GitLab)

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http://gitlab.nektar.info

# What development practices support a large multi-plaform collaborative software project such as Nektar++?

- Version-con
- Issue tracki GitLab Community Edition

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#### Open source software to collaborate on code

Manage git repositories with fine grained access controls that keep your code secure. Perform code reviews and enhance collaboration with merge requests. Each project can also have an issue tracker and a with it

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nektar.info

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README.md

#### Nektar++

Nektar++ is an open-source software framework designed to support the development of high-performance scalable solvers for partial differential equations (PDEs) using the spectral/hp element method.

This package consists of a set of libraries (the framework) and a number of pre-written PDE solvers for a selection of application domains.

The software and User Guide is available for download from http://www.nektar.info/.

#### What development practices support a large multi-plaform



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#### Tests & Continuous Integration (Buildbot) http://buildbot.nektar.info

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### http://gitlab.nektar.info

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### ulti-plaform ar++?

#### lab.nektar.info:

#### bot.nektar.info

BuildBot (0.8.9) working for the Nektar++ project Page built: Mon 22 Jun 2015 11:10:04 (BST)



BuildBot (0.8.9) working for the Nektar++ project Page built: Mon 22 Jun 2015 11:10:04 (BST)

#### Builder Ubuntu 12.04 64-bit (full) Build #659

#### Results:

#### Failed tests

#### SourceStamp:

Branch	feature/threading
Got Revision	3176edb8fc5bc697a832c660ff0d64662963566d

#### BuildSlave:

ubuntu-12 04

#### Reason:

A build was forced by 'Chris':

#### Steps and Logfiles:

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#### **Build Properties:**

Name	Value	Source
branch	feature/threading	Build
builddir	/home/buildbot/nektar/slave/ubuntu-12_04-full	slave
buildername	Ubuntu 12.04 64-bit (full)	Builder
buildnumber	659	Build
codebase		Build
got_revision	3176edb8fc5bc697a832c660ff0d64662963566d	Git
ncpus	2	BuildSlave
owners	[u'Chris']	A build was forced by 'Chris':
project		Build
repository		Build
revision		Build
scheduler	force	Scheduler
slavename warnings-count workdir	ubuntu-12_04 1 /home/buildbot/nektar/slave/ubuntu-12_04-full	BuildSlave WarningCountingShellCommand slave (deprecated)

#### **Forced Build Properties:**

Name	Label	Value
force build clean	Force a make clean	False
owner		Chris
reason		
url_suffix	Suffix to repo url	nektar/nektar.git
wipe_build	Completely wipe build directory	False

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#### Responsible Users:

no responsible users

#### Timing:

Start	Tue Jun 9 12:34:01 2015
End	Tue Jun 9 15:40:44 2015
Elapsed	3 hrs, 6 mins, 42 secs

#### **Resubmit Build:**

To force a build, fill out the following fields and push the 'Force Build' button

Reason for re-r	unning build:
Rebuild using:	Exact same revisions
Rebuild	



### nektar.info

No service of the second	

#### aform Builder Ubuntu 12.04 64-bit (full) Build #659 Results: **Build Properties:** Name Value Source Failed tests branch feature/threading Ruild /home/buildbot/nektar/slave/ubuntu-12 04-full SourceStamp: buildername Ubuntu 12.04 64-bit (full) codebase Branch feature/threading 3176edb8fc5bc697a832c660ff0d64662963566d got revision 3176edb8fc5bc697a832c660ff0d64662963566d Got Revision [u'Chris'] A build was forced by 'Chris' owners BuildSlave: project repository ubuntu-12 04 (view as text) Reason: ctest -12 '--timeout 600' --output-on-failure in dir /home/buildbot/nektar/slave/ubuntu-12 04-full/build/builds (timeout 1200 secs) A build was forced by 'Chris': watching logfiles {} argv: ['ctest', '-i2', '--timeout 600', '--output-on-failure'] Steps and Logfiles: environment: HOME=/home/buildbot LANG=en GB.UTF-8 nit undate LANGUAGE=en\_GB:en LOGNAME=buildbot ure 'cmake -DCMAKE BUILD TYPE:STRING=Debug MAIL=/var/mail/buildbot PATH=/opt/local/bin:/opt/local/lib/openmpi/bin:/usr/lib/openmpi/bin:/usr/lib64/openmpi/bin:/usr/lib64/mpi/gcc/openmpi/bin PWD=/home/buildbot/nektar/slave/ubuntu-12\_04-full/build/builds SHELL=/bin/sh TERM=linux 2. warnings (1) USER=buildbot stall compile (1 mir XDG SESSION COOKTE=204222634a5a369277e2004500000003-1423328811.240864-1156323198 using PTY: False Test project /home/buildbot/nektar/slave/ubuntu-12 04-full/build/builds ests 'ctest -i2 ...' failed (1 hrs. 30 mir Start 437: APESolver APE 3DPulse WeakDG MODIFIED stdic Start 438: APESolver APE 3DPulseWall WeakDG MODIFIED 1/463 Test #438: APESolver APE 3DPulseWall WeakDG MODIFIED ..... Passed 201,29 sec Start 163: IncNavierStokesSolver bfs tg 2/463 Test #437: APESolver\_APE\_3DPulse\_WeakDG\_MODIFIED ..... Passed 349.90 sec Start 188: IncNavierStokesSolver\_Cyl\_AdaptiveSFD 3/463 Test #163: IncNavierStokesSolver\_bfs\_tg ..... Passed 152.24 sec Start 459: MeshConvert\_StarTec/StraightRW 4/463 Test #459: MeshConvert\_StarTec/StraightRW ..... Passed 123.47 sec Start 202: IncNavierStokesSolver bfs to par 5/463 Test #188: IncNavierStokesSolver Cvl AdaptiveSFD Passed 131.09 sec Start 252: ADRSolver Advection3D m12 DG hex VarP 6/463 Test #252: ADRSolver\_Advection3D\_m12\_DG\_hex\_VarP ..... 89.24 sec Start 357: ADRSolver Advection3D m12 DG hex VarP par 7/463 Test #202: IncNavierStokesSolver bfs tg par Passed 113.37 sec Start 190: IncNavierStokesSolver ChanFlow 3DH2D FFT 8/463 Test #357: ADRSolver Advection3D m12 DG hex VarP par ..... 75.62 sec Start 148: IncNavierStokesSolver ChanFlow 3DH2D MVM 9/463 Test #190: IncNavierStokesSolver\_ChanFlow\_3DH2D\_FFT ..... Passed 68.67 sec Start 144: IncNavierStokesSolver ChanStability 10/463 Test #144: IncNavierStokesSolver\_ChanStability ..... Passed 39.79 sec Start 435: APESolver APE 2DPulseWall WeakDG MODIFIED 11/463 Test #148; IncNavierStokesSolver ChapFlow 3DH2D MVM

What development practices support a large multi-plaform collaborative software project such as Nektar++?

- Version-control (Git + GitLab)
- Issue tracking (GitLab)

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Tests & Continuous Integration (Buildbot) http://buildbot.nektar.info

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Documentation (PDF + doxygen)

### http://doc.nektar.info

### http://gitlab.nektar.info
Previous model and problems:

- · New features and fixes continuously merged into master
- Code releases every 6 months 1 year
- New features constantly introducing instability

New approach:

- New features are continuously merged into master
- Bug fixes are additionally merged into a separate release branch
- More frequent patch releases
- Should remain stable and bug fixes are distributed quicker

• Release version number **V4.3.1** Maior Minor Patel

Major . Minor . Patch

Time



• Release version number v4.3.1

Major . Minor . Patch

• Primary development in 'master'





• Release version number



Major . Minor . Patch

- Primary development in 'master'
- Major/Minor releases tagged in 'master'
- Create 'release' branch



- Release version number
  V4.3.1
  Major . Minor . Patch
- Primary development in 'master'
- Major/Minor releases tagged in 'master'
- Create 'release' branch
- Bug-fixes applied in branch and merged into 'master' as normal



- Release version number
  V4.3.1
  Major . Minor . Patch
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- Cherry-picked into 'release' branch



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  Major . Minor . Patch
- Primary development in 'master'
- Major/Minor releases tagged in 'master'
- Create 'release' branch
- Bug-fixes applied in branch and merged into 'master' as normal
- Cherry-picked into 'release' branch
- Monthly patch releases

- 1. New code is committed to a branch in git
  - feature/[name] for new functionality
  - fix/[name] for bug fixes
  - tidy/[name] code formatting updates (no functional change)
  - ticket/[number]-[description] for resolving specific issues

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  - Typically two reviewers for new features
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  - Typically one reviewer for smaller fixes
- 5. Reviewers suggest any changes or improvements, verify code meets *contribution criteria* and *code guidelines*, etc.
- 6. Iterate between authors and reviewers until everyone happy.
- 7. Senior developer performs the merge.

# **Review Process: Contribution criteria**

Some of the key aspects required include:

- Documentation
  - Has new user-exposed features been documented in the user guide?
  - Have any relevant tutorials been updated?
  - Do new functions/classes include doxygen documentation?
  - Is the code sensibly commented?
- Testing
  - Have regression tests been added for new features?
  - Do existing regression tests all pass on buildbot?
- Formatting according to coding guidelines
  - 80 char width, indentation of 4 spaces, no tabs, no namespace indentation
  - All code blocks should use braces, braces on new lines
  - Avoid preprocessor directives where possible
  - Spaces around operators, after if, while, etc
- Appropriately updated the CHANGELOG

# Further information, and What's Next?

Further information

- http://www.nektar.info
- Nektar++: An open-source spectral/hp element framework,
  C. D. Cantwell, D. Moxey, A. Comerford, et al.,
  Computer Physics Communications, vol.192, p205–219, 2015

What's Next?

- Expand tutorials
- Developer's Guide
- Packaged binaries for Windows