# BATH HPCBYTES

#### ISSUE 5

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Alex Doak is an EPSRC National Fellow in Fluid Dynamics (NFFDy), working in the Department of Mathematical Sciences (grant number EP/X028607/1). He works on a variety of problems related to nonlinear dispersive waves arising in fluid dynamical contexts.

n the ocean and atmosphere, vertical variations in temperature and salinity stratify the water column. These variations in density allow for the formation and propagation of so-called "internal gravity waves". Compared to surface waves one may be familiar with during a day out at the beach, they can be of very large amplitude (in the order of hundreds of metres). Internal waves are generated by both wind forcing on the oceans surface and tidal effects interacting with underwater bathymetry. They are responsible for considerable momentum, mass, energy, and bio-matter transport [1], and further understanding of them aids in their parametrisation in global ocean models.

Alex is interested in what are known as solitary waves: waves of infinite wavelength such that they are com-

"Alex has benefited from running multiple parallel jobs on Nimbus, which is essential for efficiently accelerating thorough parameter sweeping."

posed of a spatially localised disturbance. During his fellowship, he is considering a stratification composed of three layers of constant density separated by two pycnoclines (regions in which water density increases rapidly with depth). He is exploring waves of the second baroclinic mode (referred to as "mode-2" waves), defined as such by their vertical structure. For mode-1 waves, the two pycnoclines go up and down together, while the opposite is true for mode-2 waves, resulting in the bulbous like waves as seen in figures 1 and 2.

In previous work [2], Alex found many steady state solutions for mode-2 solitary







Figure 1: Density field of a simulation. The initial lock release is shown in the left panel. The right panel shows the generated wave, where the black curves show the location of the pycnoclines of a steady state solution. The wave is unstable, due to energy loss through a resonant tail.



Figure 2: The left panel shows the density field of a lock-release simulation. The black curves show the location of the pycnoclines of a steady state solution. The right panels compare the magnitude of the velocity field |U| for the SPINS simulation and the steady state solution.

waves, recovered by assuming that the waves propagate at constant speed and unchanging in form. The solution space is very rich, with phenomena such as multiplicity of solutions (more than one solution with the same speed) and embedded solitary waves, which are solitary waves which travel at the same speed as finite wavelength linear waves. The existence of these steady state solutions, however, does not guarantee their physical relevance. In particular, what remains unknown is their sta-

bility (can they travel large distances unchanged?) and potential generation mechanisms (can the waves be formed in

laboratory and field conditions?).

While steady states can be computed using his personal laptop, time-dependent codes are more computationally expensive, and hence Alex has been using the Nimbus HPC facilities to explore these questions. He is using the SPINS (Speudospectral Incompressible Navier-Stokes) solver [3] to integrate the twodimensional Navier-Stokes equations. As a initial condition, he uses a numerical lockrelease to replicate a commonly used experimental set-up [4]. These computations are very small when compared with threedimensional turbulence models, and so the 4-core, 8-core, and 16-core Fsv2-series are being used for this purpose. Despite being relatively small simulations (several hours when run parallel over 16 cores), the ability to run multiple jobs at the same time is essential for parameter sweeping, due to the size of the parameter space.

The results thus far are very promising. A variety of exotic mode-2 waves have been generated through lock-release, and comparison with steady state solutions is superb. In figure 1 and 2, we show two generated solitary waves. The wave in figure 1 is an unstable embedded wave, where resonant tail causes a loss of energy in the leading wave. Meanwhile, the wave in figure 2 is a "breather", a time-periodic wave which oscillates between three different solitary waves, a consequence of the aforementioned multiplicity of solutions.

#### References

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# Python Package Installation in User Area on Nimbus

Rather than installing software system-wide, wouldn't it be great if we could install python package dependencies separately for each project specific application. With frequent updates in the Python library packages, managing the dependencies with support from HPC Admin would not be an effective approach to follow. Conda package manager allows us to manage the dependencies independently in userspace without the need for admin privileges. Users can create as many projectspecific environments as needed on Nimbus in their areas without admin privileges and easily activate or deactivate environments to switch between them.

### Steps to Build a Python Environment: A Demonstration

Imagine you have a Python code for a research problem that requires more than 48 hours to run a single simulation. You have discovered that "numba" a Python compiler, could potentially speed up the simulation. Now, your goal is to install numba without affecting the existing packages you are already using for the simulation.

#### Step-1: Submit an interactive job from your Nimbus account to create the environment

```
# Change account and partition as per your account and allocation.
[user@nimbus-1-login-1~]$ srun --account=CA-CS1HGN-015 --qos=spot-fsv2-2 --nodes=1 --ntasks-per
-node=1 --partition=spot-fsv2-2 --time=01:00:00 --pty bash
```

# This will lend you on a compute node for 1 hr. user@nimbus-1-spot-fsv2-2-pq0-2~\$

#### Step-2: Creating the Environment and Installing the required packages in the active interactive session

```
# Use miniconda module for creating the environment.
user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ module purge
user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ module load Miniconda3/4.9.2
# Specify the directory to store the environment (Choose your own directory here)
user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ export CONDA_ENVS_PATH=/campaign/CA-CS1HGN-015/envs
user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ conda create --name numba-test
# You may need to initiate the base environment first before activating the created environ-
ment
user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ source /shared/home/user/.bashrc
(base) user@nimbus-1-spot-fsv2-2-pq0-2 ~ $ conda activate numba-test
(numba-test)user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ conda install numba
# Check the installed package
(numba-test)user@nimbus-1-spot-fsv2-2-pg0-2 ~ $ conda list | grep numba
                          0.59.1
numba
                                                 pypi 0 pypi
```

Step-3: Exit the interactive job and submit a batch job using the created environment

# Use the following command in your jobscript to activate the env to use numba for your job conda activate /campaign/CA-CS1HGN-015/envs/numba-test

## **HPC News and Updates**

#### Isambard 3 Update

- Isambard 2 Phase 3 cluster (A100s,M100s,and AMD Milan nodes) in maintenance from 4th June.

- Users must move important data off Isambard 2.

#### Nimbus Training Announcement

- Join us for the Interactive Computing training with Jupyter Notebook on 18th June. Register with link: https://forms.office.com/e/D6tYMVSTLq

## <u>Tip of the Month</u> To Get the Details of a Specific Module

# To see the list of available modules
[user@login1 ~]\$ module avail -1
# Display the specific module details
[user@login1 ~]\$ module show mkl/mkl-2021.1

# This will display the PATHs of libraries and executables within the module file.

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