Oasis - User Manual

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Oasis (Optimized And StrIpped Solver) is a high-performance Navier-Stokes solver written entirely in the Python interface to FEniCS. The solver is unstructured, runs with MPI and interfaces, through FEniCS, to state-of-the-art linear algebra backends like PETSc and Trilinos.

To be able to work with *Oasis*, a user should posess basic skills in how to solve PDEs through FEniCS, that in turn requires basic programming skills in Python. A good introduction to the FEniCS and *dolfin*, which is the problem solving environment of FEniCS, can be obtained by following the tutorial: http://fenicsproject.org/documentation/tutorial.

1 Installation

Oasis may be installed using the git version control system or by downloading released packages. Oasis depends on FEniCS (fenicsproject.org) and the development version of Oasis will at all times attempt to stay compatible with the development version of FEniCS. When a release is made for FEniCS, then a release will be made for Oasis as well. Oasis will not run with an incompatible version of FEniCS.

1.1 Dependensies (FEniCS)

FEniCS is installed by following instructions from the page http://fenicsproject.org/download/. There are binary packages for all FEniCS releases that can be installed easily for most operating systems (except Windows). If you want to use the development version of *Oasis*, then you need to install development version of FEniCS from source. This is quite a demanding task, unless it is performed through dorsal (see link on FEniCS download page).

1.2 Installation of *Oasis* through *git*

Oasis can be installed simply by cloning the github repository to your own computer

- \$ git clone https://github.com/mikaem/Oasis.git
- \$ cd Oasis

No further installation is necessary and the clone will leave you on the *master* branch of *Oasis*. You may now choose to switch branch or to check out a previous release. A list of remote tags is obtained with

```
$ git ls-remote tags
```

which at the time of writing results in two tags:

The 1.3.0 tag represents a release of Oasis that is compatible with version 1.3.0 of dolfin. It is obtained though

```
$ git checkout 1.3.0
```

Note that you will not have write access to the remote repository at https://github.com/mikaem/Oasis.git and as such you cannot push the changes you make to this repository. If you intend to develop and commit code yourselves, you probably want to create a fork of the *Oasis* repository by pressing the **Fork** button on github (you need to be a registered user on github). Proceed by cloning this fork to your own computer and start working on a new branch. For example, to start a new branch using the tag of *Oasis* that is compatible with fenics 1.3.0, you can execute the following commands after forking (with user name on github 'github-username')

```
$ git clone https://github.com/github-username/Oasis.git
$ git checkout -b newbranch 1.3.0
$ ... make changes
$ git commit -a -m "Some_changes"
$ git push --set-upstream origin newbranch
```

1.3 Installation of *Oasis* by downloading released version

Oasis may also be installed without git by downloading and extracting a released version from https://github.com/mikaem/Oasis/releases. To install a version of Oasis that is compatible with fenics version 1.3.0, you can execute the following commands

```
$ wget https://github.com/mikaem/Oasis/archive/1.3.0.tar.gz
$ tar -xvf 1.3.0.tar.gz
$ cd Oasis-1.3.0
```

This version of the solver will be detached from the main repository, though, and may not be kept up to date with the development version.

2 Files and folders

Oasis is designed as a Python package with a main executable module (NSfracStep.py) and three submodules (common, solvers, problems). Oasis consists of all files and folders

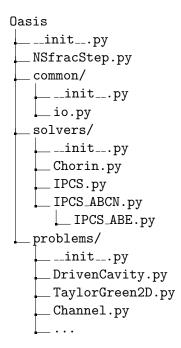


Figure 1: Directory tree structure of *Oasis*.

shown in Figure 1.

2.1 NSfracStep.py

The main module NSfracStep.py is executable and requires only that the problem to be solved is added after the keyword problem

\$ python NSfracStep.py problem=DrivenCavity solver=IPCS_ABCN or the preferred way through Ipython

[1] run NSfracStep problem=DrivenCavity

The solver keyword is optional since IPCS_ABCN is the default solver (IPCS is short for incremental pressure correction). The NSfracStep module pulls in required information from one solver module in the solvers subfolder and one problem in the problems subfolder. The required information from the problem module is a computational mesh, initial and boundary conditions, control parameters plus any other user defined action. A user should not need to do modify anything in common or solvers submodules and is only required to create a problem module.

The NSfracStep module contains a high-level implementation for a generic fractional step algorithm for the Navier-Stokes equations. The most significant part of the implementation is shown in Figure 2. All functions have default implementations in the common, solvers or problems submodules. Most interesting for users are functions ending in hook, that may be overloaded in the problem module. For example, the function

start_timestep_hook is called at the start of every new time step and may as such be used to update, e.g., a time dependent boundary condition.

The NSfracStep module is responsible for creating function spaces, test and trial spaces as well as allocating functions to hold the actual finite element solution. The most important variables declared in the module are shown in Fig. 3.

2.2 problems

The problems submodule contains files

- __init__.py default implementation of all hook functions and default parameters.
- Channel.py Turbulent channel flow test problem in 3D.
- DrivenCavity.py Lid driven cavity test problem in 2D.
- LaminarChannel.py Laminar flow in a 2D channel with a constant applied pressure gradient. Starting from rest.
- Lshape.py Laminar flow in a 2D L-shaped domain driven by varying the pressure on one of two inlet/outlets in time.
- TaylorGreen2D Taylor Green flow. Doubly periodic test problem in 2D.
- TaylorGreen3D.py Taylor Green flow. Triply periodic test problem in 3D.

The default version of all hook functions are implemented in module problems/__init__.py as shown in Figure 4. Any function may be overloaded by reimplementing it in the user defined problem module.

Note the special calling sequence for the functions used in Fig. 2 and declared in Fig. 4. The functions are called with the entire NSfracStep namespace **vars() as argument and in the declaration of the function (Fig. 4) any variable required may be unpacked in the list of arguments and used by reference inside the function. There is no copying involved and the overhead in calling functions this way is very small, yet extremely flexible.

Control parameters The problems/__init__.py module contains a range of control parameters that may be overloaded by the user. The control parameters are kept in a dictionary called NS_parameters, as shown in Fig. 5. The purpose of each parameter is also hinted at in Fig. 5. Output of results to file is controlled by parameters checkpoint, save_step, folder and output_timeseries_as_vector. The folder variable is a string giving the name of the main folder used for storage. Using default value folder = "results", the results will be stored in folder Oasis/results/data/ in a directory tree similar to that shown in Fig. 6. To avoid accidentally overwriting old results, each new execution of the program creates a new folder with a unique integer under the data folder unless the solver is restarted from a previous solution. In that case, the same folder is used

```
# Preassemble and prepare solver
vars().update(setup(**vars()))
# Anything problem specific
vars().update(pre_solve_hook(**vars()))
# Enter loop for time advancement
while t < T and not stop:
 t += dt
 inner_iter = 0
  # Do something at start of timestep
  start_timestep_hook(**vars())
  # Enter velocity/pressure inner loop
  for inner_iter < max_iters:</pre>
   inner_iter += 1
    if inner_iter == 1:
      assemble_first_inner_iter(**vars())
    # Solve tentative velocity
    for i, ui in enumerate(u_components):
      velocity_tentative_assemble(**vars())
      velocity_tentative_hook (**vars())
      velocity_tentative_solve
                                 (**vars())
    # Solve pressure correction
   pressure_assemble(**vars())
    pressure_hook (**vars())
                     (**vars())
   pressure_solve
  # Solve velocity update
 velocity_update(**vars())
  # Solve for all scalar components
  if len(scalar_components) > 0:
    scalar_assemble(**vars())
    for ci in scalar_components:
      scalar_hook (**vars())
      scalar_solve(**vars())
  # Do something at end of timestep
 temporal_hook(**vars())
  # Save and update to next timestep
  stop = save_solution(**vars())
# Finalize solver
theend_hook(**vars())
```

Figure 2: The fractional step time integration algorithm in NSfracStep.py

```
# Declare function spaces and trial and test functions
V = FunctionSpace(mesh, "Lagrange", velocity_degree)
Q = FunctionSpace(mesh, "Lagrange", pressure_degree)
u, v = TrialFunction(V), TestFunction(V)
p, q = TrialFunction(Q), TestFunction(Q)
# Get dimension of problem
dim = mesh.geometry().dim()
# Create list of components we are solving for
u_components = map(lambda x: "u"+str(x), range(dim))# velocity components
uc_comp = u_components + scalar_components # velocity + scalars
sys_comp = u_components + ["p"] + scalar_components # velocity +
   pressure + scalars
# Create dictionaries for the solutions at three timesteps
q_ = {ui: Function(V) for ui in uc_comp}
q_1 = {ui: Function(V) for ui in uc_comp}
q_2 = {ui: Function(V) for ui in u_components} # Note only velocity
# Allocate solution for pressure field and correction
p_{-} = q_{-}["p"] = Function(Q)
phi_ = Function(Q)
# Create vector views of the segregated velocity components
u_ = as_vector([q_ [ui] for ui in u_components])# Velocity vector t
u_1 = as_vector([q_1[ui] for ui in u_components]) # Velocity vector t-dt
u_2 = as_vector([q_2[ui] for ui in u_components]) # Velocity vector t-2*dt
```

Figure 3: The declaration section of NSfracStep.py. Allocation of necessary storage and parameters for solving the momentum equation through its segregated components. FunctionSpace, Function, TrialFunction, TestFunction, as_vector are all classes or functions imported from the dolfin module.

and new results are appended to those already existing. The Checkpoint folder contains all parameters (NS_parameters) and solution vectors stored in HDF5 format, that are continuously overwritten every checkpoint time step. The solution vectors in the Checkpoint folder contain the velocity at two previous time steps and the pressure from the latest, thus making it possible to stop and restart the solver from this solution at no loss of accuracy whatsoever. The TimeSeries folder contains solution files in dolfin's XDMF-HDF5 format, viewable by, e.g., the external visualisation tool Paraview (paraview.org). Results are stored every save_step time step and the velocity is stored as a vector and not three (or two) scalars. This exact behaviour may be altered by setting NS_parameters["output_timeseries_as_vector"] = False. The remaining folders in Fig. 6 are empty unless explicitly coded in the problem module, see, e.g., problems/Channel.py. The Stats folder contains turbulence statistics, whereas the Voluviz folder contains fields possible to view with Voluviz, an in-house visualisation tool developed at the Norwegian Defence Research Establishment (FFI), available upon request from the authors.

```
def body_force(mesh, **NS_namespace):
    """Specify body force"""
    return Constant((0,)*mesh.geometry().dim())
def scalar_source(scalar_components, **NS_namespace):
    """Return a dictionary of scalar sources."""
    return dict((ci, Constant(0)) for ci in scalar_components)
def initialize(**NS_namespace):
    """Initialize solution."""
    pass
\operatorname{def} create_bcs(sys_comp, **NS_namespace):
    """Return dictionary of Dirichlet boundary conditions."""
    return dict((ui, []) for ui in sys_comp)
\mathbf{def} velocity_tentative_hook(**NS_namespace):
    """Called just prior to solving for tentative velocity."""
    pass
def pressure_hook(**NS_namespace):
    """Called prior to pressure solve."""
    pass
def scalar_hook(**NS_namespace):
    """Called prior to scalar solve."""
\operatorname{def} start_timestep_hook(**NS_namespace):
    """Called at start of new timestep"""
    pass
def temporal_hook(**NS_namespace):
    """Called at end of a timestep."""
\operatorname{def} pre_solve_hook(**NS_namespace):
    """Called just prior to entering time-loop. Must return a
   dictionary."""
   return {}
def theend_hook(**NS_namespace):
    """Called at the very end."""
    pass
```

Figure 4: All problem specific functions defined in problems/__init__.py that may be overloaded in the implemented problem module. The dictionary NS_namespace is the namespace of the NSfracStep module.

```
NS_parameters = dict(
 # Physical constants and solver parameters
                        # Kinematic viscosity
 nu = 0.01,
 t = 0.0,
                        # Time
 tstep = 0,
                        # Timestep
                        # End time
 T = 1.0,
 dt = 0.01,
                        # Time interval on each timestep
 # Some discretization options
  # Use Adams Bashforth projection to estimate pressure on new time step
 AB_projection_pressure = False,
 velocity_degree = 2,
 pressure_degree = 1,
 solver = "IPCS_ABCN", # "IPCS_ABCN", "IPCS_ABE", "IPCS", "Chorin"
 # Parameters used to tweek solver
 max_iter = 1,
                        # Number of inner pressure velocity iterations
                    # Tolerance for inner iterations
 max_error = 1e-6,
 iters_on_first_timestep = 2,# Number of iterations on first timestep
 use_krylov_solvers = False, # Otherwise use LU-solver
 low_memory_version = False, # Use assembler and not preassembled mat.
 print_intermediate_info = 10,
 print_velocity_pressure_convergence = False,
 velocity_update_type = "default", # "gradient_matrix" , "lumping"
  # Parameters used to tweek output
 plot_interval = 10,
  checkpoint = 10, # Overwrite Checkpoint results each checkpoint tstep
                    # Store solution in new folder each save_step
  save_step = 10,
                       # Relative folder for storing results
 folder = 'results',
 restart_folder = None, # If restarting solution, set the folder
   holding the solution to start from here
  output_timeseries_as_vector = True, # Use Velocity vector in Timeseries
  # Solver parameters transferred to dolfin's parameters['krylov_solver']
 krylov_solvers = dict(
   monitor_convergence = False,
   report = False,
   error_on_nonconvergence = False,
   nonzero_initial_guess = True,
   maximum_iterations = 100,
   relative_tolerance = 1e-8,
   absolute_tolerance = 1e-8)
# For periodic domains recreate constrained_domain in problem module
constrained_domain = None
# To solve for scalars provide a list like ['scalar1', 'scalar2']
scalar_components = []
# Diffusivities: Schmidt = nu/D (momentum diffusivity / mass diffusivity)
Schmidt = defaultdict(lambda: 1.)
```

Figure 5: Control parameters for solver.

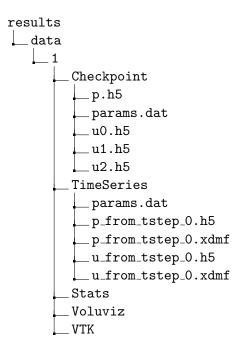


Figure 6: Directory tree structure of results stored by *Oasis*.

Note that computing turbulence statistics and Voluviz-fields require the Python package fenicstools (https://github.com/mikaem/fenicstools).

2.3 solvers

The solvers submodule contains specific implementations of fractional step algorithms.

- __init__.py Default (empty) implementation of most functions seen in Fig. 2 (serves as a base module).
- Chorin.py Naive implementation of Chorin's projection method. Adams-Bashforth advecting velocity and Crank-Nicolson for diffusion and advected velocity.
- IPCS.py A naive implementation of the incremental pressure correction scheme using Adams-Bashforth advecting velocity and Crank-Nicolson for diffusion and advected velocity. The scheme is second order in time.
- IPCS_ABCN.py Optimized implementation of IPCS.
- IPCS_ABE.py Optimized implementation using explicit Adams-Bashforth convection.

The functions implemented in the solvers submodule cannot be overloaded by the user in the problem module.

2.4 common

The common folder contains two files:

- __init__.py contains one single function, parse_command_line that is used to parse any parameters supplied through the command line.
- io.py contains functions for storing and retrieving solutions.
 - save_solution used for storing intermediate or checkpoint solutions.
 - create_initial_folders used for creating the folders storing results (see Fig.6).
 - check_if_kill checks if a file named killoasis has been placed in the NS_parameters['folder'] directory. If found, then the solver is stopped cleanly at the end of the time step after saving the solution to the Checkpoint folder.
 - init_from_restart used for restarting the solver from a previously stored solution in Checkpoint folder.

3 Implementing a new problem

Oasis is a programmable solver and the user is required to implement new problems by creating a new Python module (a file ending in .py) located in the *problems* folder. A problem module must implement at least

- A dolfin Mesh.
- Boundary conditions.
- Control parameters, e.g., viscosity, time step and end time.

And for most problems you will probably also want to set

- Initialisation of the solution. (dolfin Functions are automatically initialised to zero).
- Post-processing.

Lid driven cavity We will now illustrate by implementing the common lid driven cavity test problem. The lid driven cavity is computed on a two-dimensional domain $\Omega = [0,1] \times [0,1]$, where the velocity of the top lid at y=1 is u=(1,0) and there is no-slip on the remaining three surrounding walls. The kinematic viscosity is 0.01 and the flow is laminar.

Start by creating a new empty file in the problems folder

```
$ touch DrivenCavity.py
```

First thing you want to do now is to import all default hook-functions and control parameters from the problems module

```
from problems import *
```

The entire namespace of problems/__init__.py is now imported into the current module. Note that this includes also the entire dolfin namespace since from dolfin import * is called from within problems/__init__.py.

Next on the todo list is to create a computational mesh. The mesh can either be created using dolfin's built in meshing capabilities or be read in from file. Furthermore, mesh may be created as a callable function or a variable name. When using built ins we usually choose to create a callable function, since this allows us to set the size of the mesh through the command line interface. The mesh is here created as a callable function using the UnitSquareMesh function from the dolfin namespace

```
from numpy import cos, pi
def mesh(Nx, Ny, **params):
    m = UnitSquareMesh(Nx, Ny)
    x = m.coordinates()
    x[:] = (x - 0.5) * 2
    x[:] = 0.5*(cos(pi*(x-1.) / 2.) + 1.)
    return m
```

The mesh is skewed towards the walls since it is important to capture the large gradients of the flow near the corners. The coordinates of the mesh are collected in the variable x, which is a numpy array of shape $((Nx+1)\cdot (Ny+1),2)$ with view into the UnitSquareMesh object. Thus, modifying x simultaneously modifies the coordinates of the mesh.

We now have a mesh and are left with control parameters and boundary conditions. Control parameters may all be set through the command line or by updating the NS_parameters dictionary (see Fig. 5)

```
# Override some problem specific parameters
NS_parameters.update(
    nu = 0.001,
    T = 1.0,
    dt = 0.001,
    Nx = 50,
    Ny = 50,
    plot_interval = 20,
    save_step = 10,
    folder = 'drivencavity_results',
    print_intermediate_info = 10,
    use_krylov_solvers = True)
```

The plot_interval parameter represents a variable that does nothing in itself. However, we will make use of it in the temporal_hook function, called at the end of each time step. Likewise, the meshing parameters Nx, Ny are specific to the DrivenCavity module and not found originally in the NS_parameters dictionary in problems/__init__.py . Note how Nx and Ny are used by the callable mesh function.

Dirichlet boundary conditions are created like for any other FEniCS application by using dolfin's DirichletBC class:

The noslip and top strings are used to identify parts of the boundary using corresponding coordinates (x, y) = (x[0], x[1]). V is the FunctionSpace of the velocity components. Note that the boundary condition for the top lid is placed first in the list for u0 (velocity component in x-direction). This has implications for the velocities in the two corners located at (x,y) = (0,1) and (x,y) = (1,1), that are now set to zero. If the boundary condition for the top (i.e., bc00) is placed last in the list, then we obtain u = (1,0) in both corners. There are no boundary conditions for the pressure.

At this point we have already specified enough to make the solver run. Still, we want to make a few more modifications by initialising the solution and by writing some routines for visualising the solution as it evolves. The solution is by default initialised to zero. Here we simply apply the boundary conditions to the solutions, such that the solution at t = 0 has a top lid with velocity (1,0):

```
def initialize(x_1, x_2, bcs, **NS_namespace):
    for ui in x_2:
        [bc.apply(x_1[ui]) for bc in bcs[ui]]
        [bc.apply(x_2[ui]) for bc in bcs[ui]]
```

Note that x_{_}, x_{_}1, x_{_}2 are dictionaries with velocity components or pressure as keys and solution vectors as values. The vectors are views into the solution Function's q_{_}, q_{_}1, q_{_}2, declared in the NSfracStep.py module (see Fig. 3).

We want to visualise the velocity as a vector and we want the figure to be updated in the same frame as the solution progresses (i.e., do not create a new figure for each time step). To this end we need a VectorFunctionSpace and a velocity vector Function uv defined and returned to the NSfracStep namespace using the pre_solve_hook function, called prior to entering the time integration loop (see Fig. 2)

```
def pre_solve_hook(mesh, velocity_degree, **NS_namespace):
    Vv = VectorFunctionSpace(mesh, 'CG', velocity_degree)
    return dict(Vv=Vv, uv=Function(Vv))
```

The Function uv may now be unpacked, updated with the new solution and plotted in the temporal_hook function. Note also the use of the plot_interval parameter that we set in the NS_parameters dictionary.

```
def temporal_hook(tstep, u_, Vv, uv, p_, plot_interval, **NS_namespace):
    if tstep % plot_interval == 0:
        uv.assign(project(u_, Vv))
        plot(uv, title='Velocity')
        plot(p_, title='Pressure')
```

Running the problem The problem runs with, e.g.,

```
[1] run NSfracStep problem=DrivenCavity Nx=100 Ny=100
```

Any parameter may be overloaded on the command-line. The expected outcome of the program is two plots, velocity vectors and pressure, that evolve during simulations. The velocity vectors are shown in Fig. 7 for time T=1.0. Furthermore, the solution will be stored to the TimeSeries folder under drivencavity_results/data/1 each 10'th time step. Hence, for 1000 time steps, there should be 100 snapshots of both velocity and pressure. These can be post-processed using ParaView, e.g., by producing a movie from the time series.

Running with MPI The solver runs with MPI at no additional effort as long as FEniCS has been installed with support for MPI (the default packages of FEniCS are compiled with MPI support). Run the program in a bash-shell using 4 CPUs with command

```
$ mpirun -np 4 python NSfracStep.py problem=DrivenCavity T=10000.0
```

The mesh will then automatically be distributed across the 4 processors. The only visible difference is that dolfin's plots will look weird because each processor plots its own mesh and solution. Visualisation with MPI is thus best performed with a post-processing tool like Paraview, using the solution stored to TimeSeries. You may suppress intermediate plots by setting plot_interval to a really large number.

Stopping the solver Since the end time has been set to T=10000.0 through the commandline, the solver will run for quite a long time. To stop it cleanly you can create an empty file called killoasis in the result folder:

```
$ touch drivencavity_results/killoasis
```

This will make sure that the solver stops only after storing the solution on the current time step to the Checkpoint folder. The solver may, as such, be restarted from this solution at a later convenience. See problems/Channel.py for a turbulence simulation, where such behaviour has been implemented.

Adding scalars Any number of scalars may be added to the solver. To add a scalar, simply add the scalar_components list to the problem namespace, like

```
scalar_compnents = ["alfa", "beta"]
```

for adding two scalars named alfa and beta. The diffusivities are specified like, e.g.,

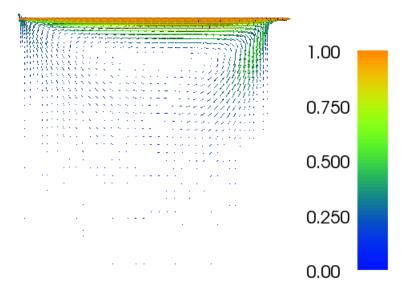


Figure 7: Driven cavity flow. Velocity vectors at T=1.0.

```
Schmidt["alfa"] = 1.
Schmidt["beta"] = 10.
```

where the Schmidt number i the momentum diffusivity divided by the mass diffusivity. Naturally, you also need to define the boundary and initial conditions. For illustration, we choose alfa=1 for y=1 and beta=1 for y=0. The create_bcs and initialize functions may to this end be extended like

```
def initialize(x_1, x_2, bcs, **NS_namespace):
   for ui in x_1:
       [bc.apply(x_1[ui]) for bc in bcs[ui]]
   for ui in x_2:
       [bc.apply(x_2[ui]) for bc in bcs[ui]]
```

Note that the scalars use the same function space as the velocity components. However, the scalars are only stored on two time steps and as such the scalars are not found in the dictionary x_2 , only x_1 and x_1 .