

A Sustainable Collaboratory for Coastal Resilience Research

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Outline

Introduction

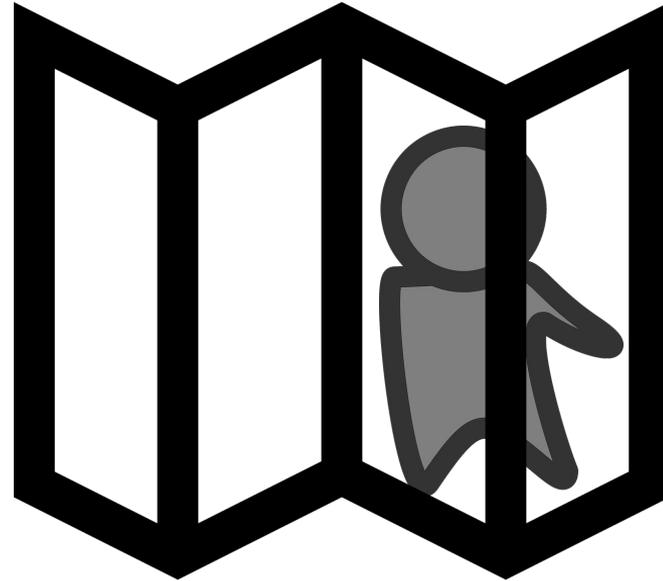
Methodology

Workflow

System

Result

Conclusion





Introduction

Goal: Create a cloud-ready repository of open-source coastal modeling tools which enable scientists and engineers to more easily use high performance computers (HPC) and to study a variety of physical and ecological processes.

We want our system to be intuitive, repeatable, collaborative



Introduction

In [2]: `import model`

Funwave-tvd

Basic Template

MGLOB: 600

NGLOB: 200

TOTAL_TIME: 30.0

PLOT_INTV: 0.2

DX: 0.05

DY: 0.10

DEPTH_OUT: T F

U: T F

V: T F

ETA: T F

Update Input File

```
!!INPUT FILE FOR BOUSS_TVD
! NOTE: all input parameter are capital sensitive
! -----TITLE-----
! title only for log file
TITLE = TEST RUN
! -----HOT START-----
HOT START =
```

The system is built upon:

1. Jupyter notebooks
2. Agave framework
3. Docker
4. Singularity



Introduction

Swan: A third-generation wave model, developed at Delft University of Technology, that computes random, short-crested wind-generated waves in coastal regions and inland waters

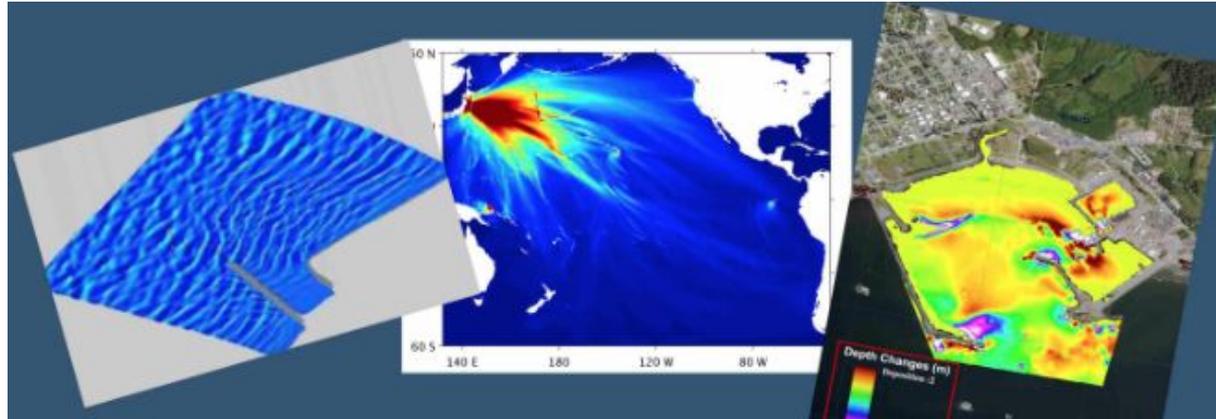
SWAN

Simulating WAves Nearshore

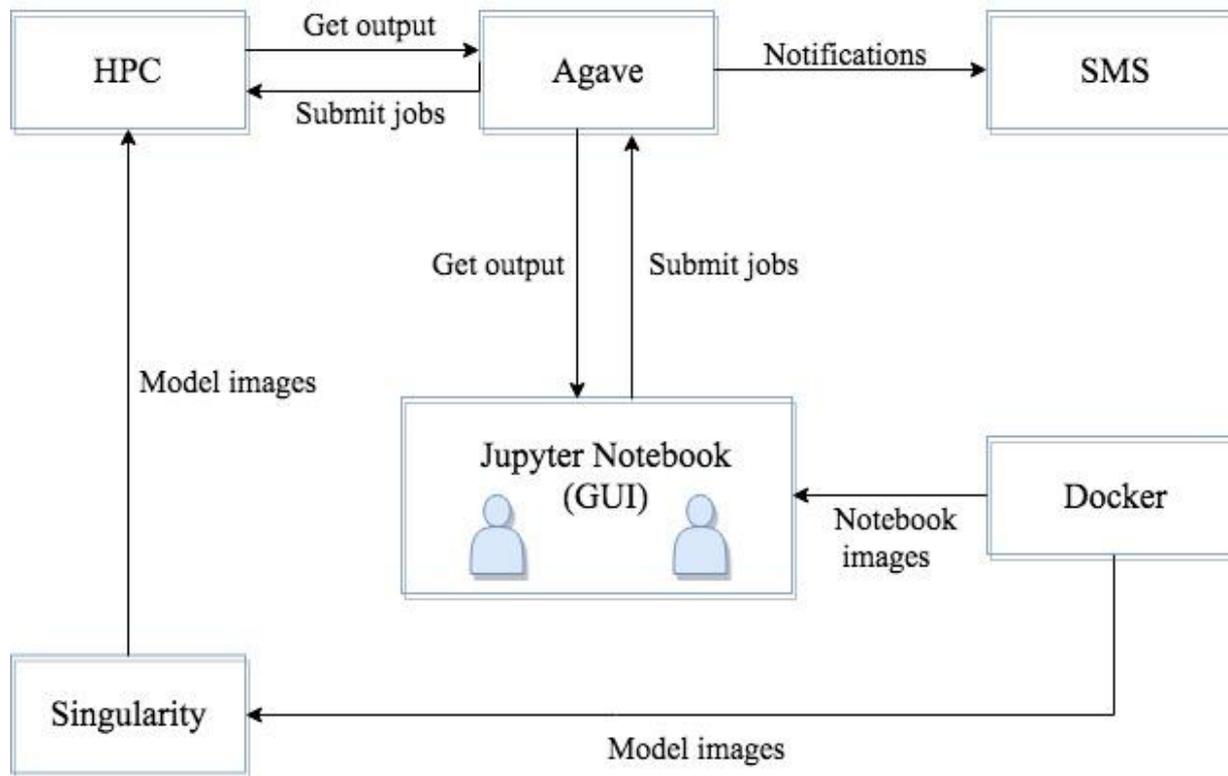


Introduction

[Funwave-tvd](#): A Boussinesq model for simulating nearshore surface-waves, currents and tsunamis from ocean-basin to nearshore scales.



Workflow





Methodology--Docker and Singularity

1. [Docker](#) is an open platform allowing developers to build, ship, and run distributed applications in self-contained environments.

Docker Hub makes it easy to share and discover images.

Security problem, not available on HPC resources.

2. [Singularity](#) makes it easy to use with MPI, and addresses the security concerns.



Methodology--Docker and Singularity

1. [Docker](#) both to construct the images for singularity and to deploy the Jupyter notebooks to use machines and workstations
2. [Singularity](#) to deploy and run simulation codes on cloud-enabled resources



Methodology--Jupyter notebook

1. [Jupyter](#) is a tool for interactive computing that is halfway between a GUI and a command-line tool
2. Create a customizable, interactive environment for science discovery and engineering analyses

Methodology--Agave platform

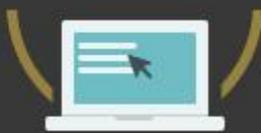


THE LEADING ALL-IN-ONE SCIENCE-AS-A-SERVICE PLATFORM FOR THE OPEN SCIENCE COMMUNITY.

MANAGE
DATA



RUN
CODE



COLLABORATE
ANYWHERE



CONNECT
ANYTHING





Methodology--Agave platform

1. [Agave](#): restful JSON API

Abstracts a way the details of the job submission process

2. Provides a detailed provenance trail.
3. Fine-grained access controls for sharing jobs and data across machine boundaries.



System--before using

- Configure machine/resource
- Configure user access
- Permissions need to be given





System--configuration

```
In [1]: import configuration2
```

```
Password or secret: AGAVE_PASSWD
Reading file `AGAVE_PASSWD.txt`
Password or secret: PBTOK
Reading file `PBTOK.txt`
```

Agave username

Execute machine

Storage system name

Project name

Configure

```
1 from agave import *
2 from ipywidgets import Box, Text, Layout, Label, Button
3
4 readpass("AGAVE_PASSWD")
5 readpass("PBTOK")
6
7 item_layout = Layout(
8     display = 'flex',
9     flex_flow = 'row',
10    justify_content = 'flex-start',
11    width = '50%'
12 )
13
14 agaveText = Text()
15 execMachineText = Text(value="shelob-exec-stevenbrandt2")
16 machineNameText = Text(value="shelob-storage-stevenbrandt23")
17 appText = Text(value="crcollaboratory-shelob-stevenbrandt2-2.0")
18 pbtokText = Text()
19 confBtn = Button(description='Configure', layout=Layout(
20     display = 'flex',
21     flex_flow = 'row',
22     justify_content = 'center',
23     width = '100px',
24     disabled=False
25 ))
26
27 def confBtn_click(a):
28     configure2(agaveText.value, execMachineText.value,
29               machineNameText.value, appText.value)
30
31 confBtn.on_click(confBtn_click)
```



System--input

In [2]: `import model`

Funwave-tvd

Basic Template

MGLOB: 600

NGLOB: 200

TOTAL_TIME: 30.0

PLOT_INTV: 0.2

DX: 0.05

DY: 0.10

DEPTH_OUT:	T	F
U:	T	F
V:	T	F
ETA:	T	F

Update Input File

```
!!INPUT FILE FOR BOUSS_TVD
! NOTE: all input parameter are capital sensitive
! -----TITLE-----
! title only for log file
TITLE = TEST RUN
! -----HOT START-----
HOT START = F
```

```
199 ##### Funwave-tvd Input tab #####
200
201 fwInputdd=Dropdown(options=['Choose Input Template','Basic Template'], value='Choose
202
203
204
205 parvals = {}
206 inputBox = Box(layout = Layout(flex_flow = 'column'))
207
208 def fw_on_change(change):
209     inputTmp = ''
210     items = []
211     if change['type'] == 'change' and change['name'] == 'value':
212         if change['new'] == 'Choose Input Template':
213             items=[]
214             inputBox.children = items
215             return
216         if change['new'] == 'Basic Template':
217             cmd("tar -zxvf input_funwave.tgz")
218             inputTmp = 'input_funwave/basic_template.txt'
219
220     with open(inputTmp,"r") as fd:
221         for line in fd.readlines():
222             g = re.search(r'(\w+)\s*=\s*${(.*?)}',line)
223             if g:
224                 for match in re.findall(r'(\w+)=("[^"]*"|'\'[^\']*\'|[\^,\n])',g.gr
225                     match[0] == 'value':
226                         label = line.split()[0]+'Label'
227                         label = Label(value = line.split()[0].upper()+":")
228                         text = line.split()[0]
229                         text = Text(value=match[1])
230                         box = line.split()[0]+'Box'
231                         box = Box([label, text],layout = Layout(width = '100%',
232                             items.append(box)
233                     if match[0] == 'option':
234                         label = line.split()[0]+'Label'
235                         label = Label(value = line.split()[0].upper()+":")
236                         togBtns = line.split()[0]
237                         togBtns = ToggleButtons(options=['T', 'F'])
238                         box = line.split()[0]+'Box'
239                         box = Box([label, togBtns], layout = Layout(width = '100
240                             items.append(box)
241
242         inputBox.children = items
243
244 fwInputdd.observe(fw_on_change)
245
246 def fwUpInput_btn_clicked(a):
247     inputTmp = ''
248     if fwInputdd.value == 'Basic Template':
```



System--customize input

```
! -----DIMENSION-----
! global grid dimension
{ Mglob = ${value=601,default=601}
  Nglob = ${value=201,default=201}

! ----- TIME-----
! time: total computational time/ plot time / screen interval
! all in seconds
{ TOTAL_TIME = ${value=30.0,default=30.0}
  PLOT_INTV = ${value=0.2,default=0.2}
  PLOT_INTV_STATION = 0.02
  SCREEN_INTV = 0.1
  HOTSTART_INTV = 360000000000.0
```

Basic Template

MGLOB:	<input type="text" value="601"/>
NGLOB:	<input type="text" value="201"/>
TOTAL_TIME:	<input type="text" value="30.0"/>
PLOT_INTV:	<input type="text" value="0.2"/>
DX:	<input type="text" value="0.05"/>
DY:	<input type="text" value="0.10"/>
DEPTH_OUT:	<input checked="" type="checkbox"/> T <input type="checkbox"/> F
U:	<input checked="" type="checkbox"/> T <input type="checkbox"/> F
V:	<input checked="" type="checkbox"/> T <input type="checkbox"/> F
ETA:	<input checked="" type="checkbox"/> T <input type="checkbox"/> F



System--run

In [2]: `import model`

Funwave-tvd

Input	Run	Output	Visualization
The number of nodes	<input type="range" value="1"/>		1
The number of Processors of each node	<input type="range" value="4"/>		4
<input type="button" value="Run"/>			

```

285 ##### Run tab #####
286 run_item_layout = Layout(
287     display = 'flex',
288     flex_flow = 'row',
289     justify_content = 'flex-start',
290     width = '50%'
291 )
292
293 numnodesSlider = IntSlider(value=0, min=1, max=8, step=1)
294 numprocSlider = IntSlider(value=0, min=1, max=16, step=1)
295
296 runBtn = Button(description='Run', button_style='primary', layout= Layout(width = '5
297
298 run_items = [
299     Box([Label(value='The number of nodes', layout = Layout(width = '350px')), numno
300     Box([Label(value='The number of Processors of each node', layout=Layout(width =
301         layout= run_item_layout),
302     Box([runBtn]),
303 ]
304
305 def modifyFWinput():
306     name_value_pairs = {
307         "PX" : str(numnodesSlider.value),
308         "PY" : str(numprocSlider.value)
309     }
310     with open("input_funwave/input_tmp.txt", "r") as tmp:
311         with open("input_funwave/input.txt", "w") as inputfile:
312             for line in tmp.readlines():
313                 g = re.match("^(PX|PY)\s*=\s*(\S+)", line)
314                 if g:
315                     name = g.group(1)
316                     if name in name_value_pairs:
317                         inputfile.write(name+" = "+name_value_pairs[name)+"\n")
318                 else:
319                     inputfile.write(line)
320             inputfile.close()
321             tmp.close()
322
323 def runfun_btn_clicked(a):
324     if (modelTitle.value == "Funwave-tvd"):
325         modifyFWinput()
326         cmd("rm -fr input")
327         cmd("mkdir input")

```



System--output

In [2]: `import model`

Funwave-tvd

Input Run **Output** Visualization

List jobs history

List job output Abort

Download

```
361 ##### Output tab #####
362
363 jobListBtn = Button(description='List jobs history', button_style='primary', lay
364
365 jobSelect = Select(layout = Layout(height = '150px', width='100%'))
366
367 jobOutputBtn = Button(description='List job output', button_style='primary', lay
368
369 abortBtn = Button(description='Abort', button_style='danger', layout= Layout(wid
370
371 outputSelect = Select(layout = Layout(height = '150px', width='100%'))
372
373 downloadOpBtn = Button(description='Download', button_style='primary', layout= La
374
375 def jobList_btn_clicked(a):
376     cout = cmd("jobs-list -l 10")
377     out1 = cout["stdout"]
378     jobSelect.options = out1
379
380 jobListBtn.on_click(jobList_btn_clicked)
381
382 def abort_btn_clicked(a):
383     g = re.match(r'^\S+', jobSelect.value)
384     if g:
385         jobid = g.group(0)
386         rcmd = "jobs-stop "+jobid
387         cmd(rcmd)
388
389 abortBtn.on_click(abort_btn_clicked)
390
391
392 def jobOutput_btn_clicked(a):
393     g = re.match(r'^\S+', jobSelect.value)
```



System--visualization

In [2]: `import model`

Funwave-tvd

Input	Run	Output	Visualization
▼ 1D			
Y_in_plots	Choose one		
► 2D			
► 3D			

```
472 ##### Funwave Visualization tab #####
473
474
475 fwYoption = Dropdown(options=['Choose one','eta','u','v'])
476 fwplotsInter = widgets.interactive(fwOneD, Y_in_plots = fwYoption)
477 fwoneDBox = Box([fwplotsInter])
478
479
480 depthBtn = Button(description='display',button_style='primary', layout
481 depthOutput = widgets.Output()
482
483
484
485 def depth Btn_clicked(a):
486     print (fw_para_pairs['Mglob'])
487     print (fw_para_pairs['Nglob'])
488     with depthOutput:
489         display(waterDepth(fw_para_pairs['Mglob'],fw_para_pairs['Nglob
490
491 depthBtn.on_click(depth Btn_clicked)
492 depthBox = Box([Label(value='Water Depth'),depthBtn],layout = Layout(w
493
494
495 depProfileN = IntSlider(value=0, min=0, max=200)
496 depProfileInter = widgets.interactive(depProfile, N = depProfileN)
497 depProfileBox = Box([Label(value='Depth Profile Snapshot'), depProfile
498
499
500
501 depProfileAnimaRange = FloatRangeSlider(value=[5,7], min=0.0, max=30,
502     description='Time period (s):',readonly
503 depProfileAnimBtn = Button(description='display',button_style='primary
504 depProfileAnimOutput = widgets.Output()
505 def depProfileAnim Btn_clicked(a):
506     anim = depProfileWithEta(depProfileAnimaRange.value[0], depProfile
507     fw_para_pairs['Mglob'],fw_para_pairs
```



System--Future Work

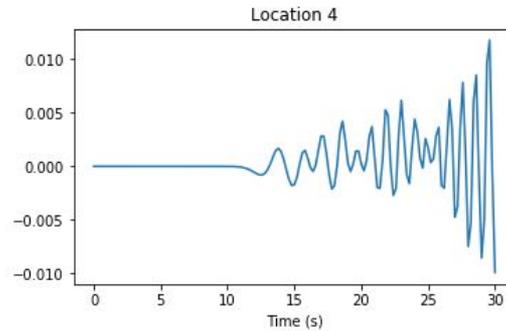
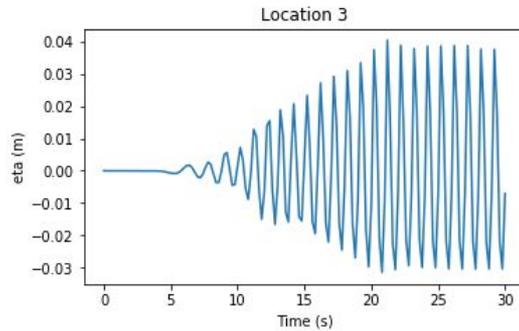
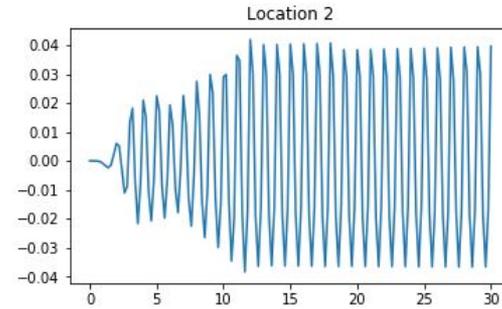
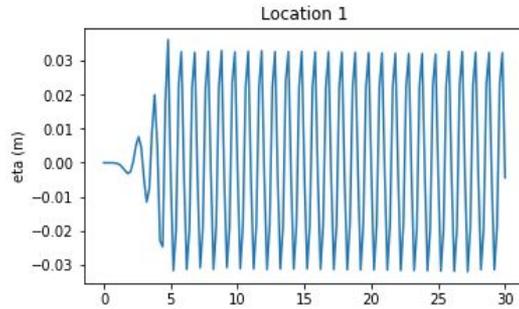
- Update OS, MPI, and source code for Funwave-tvd or Swan once a month, automatically (in progress).
- Intend to add more models
-



Results--1D

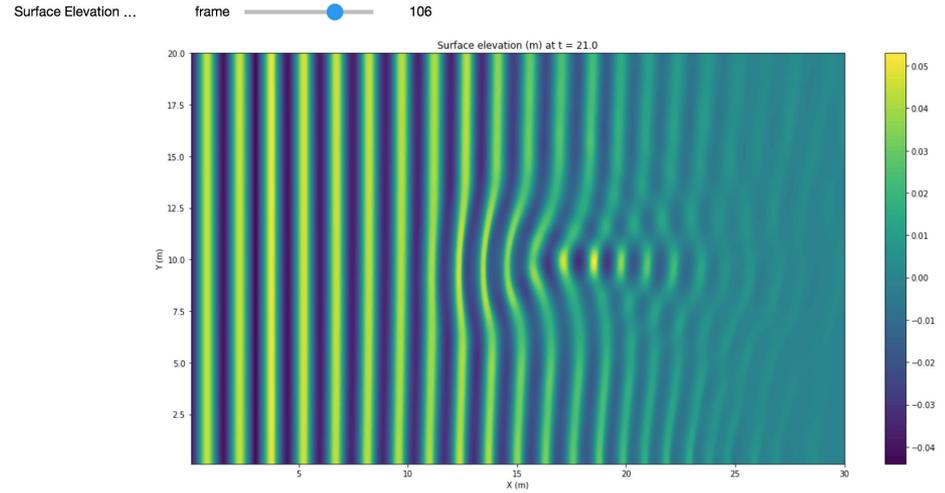
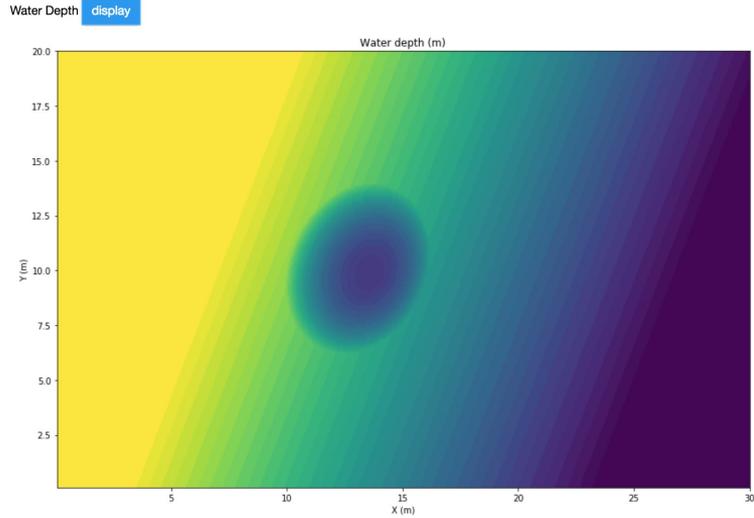
▼ 1D

Y_in_plots eta ▼





Results--vertical 2D

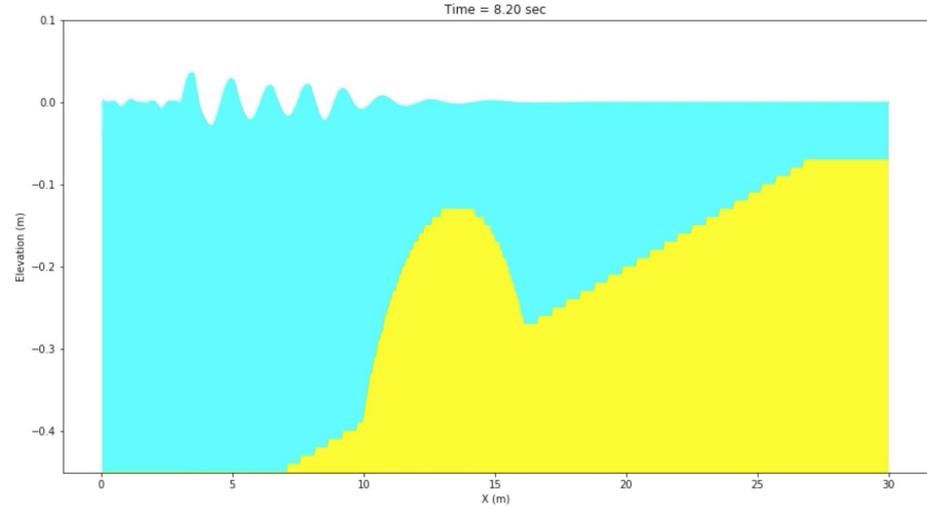
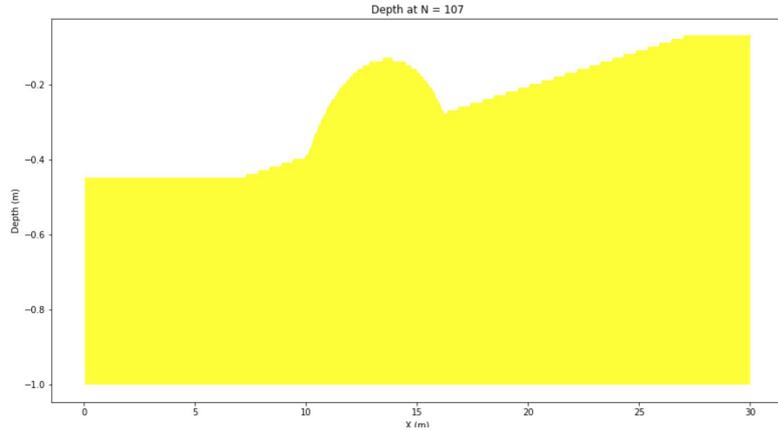




Results--horizontal 2D

Cross-shore profile animation Time perio...

Depth Profile Sna... N 107





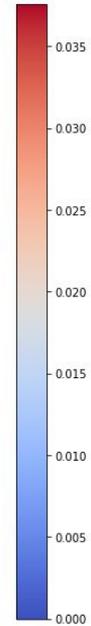
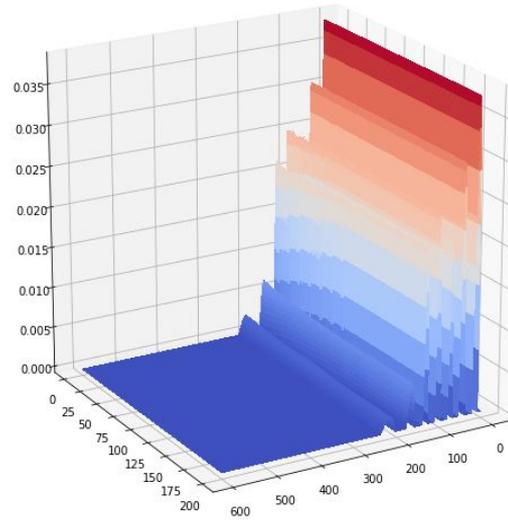
Results--3D

Surface Elevation snapshot

frame



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Conclusion

The CMR (Coastal Model Repository)

is targeting cloud and cloud-like architectures to enable quick deployment of coastal models and their working environment

serve as a community repository for precompiled open source models that are widely used by coastal researchers

Thanks!

