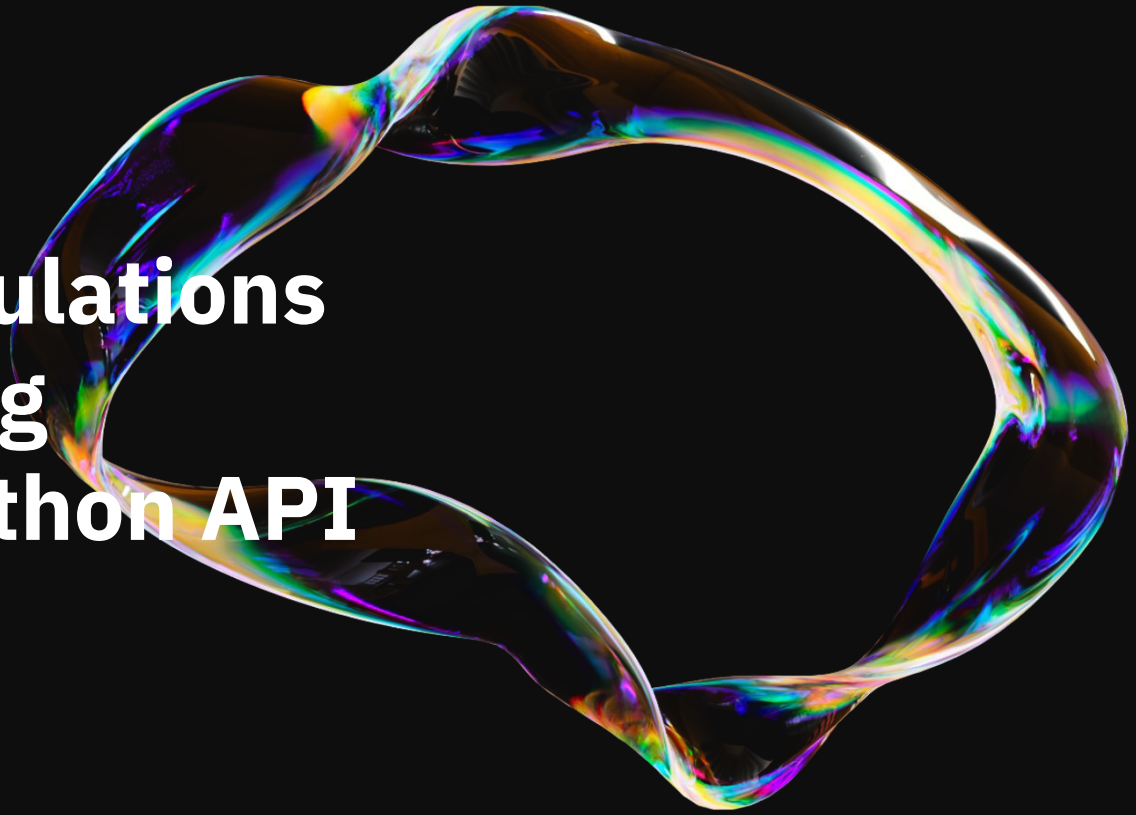
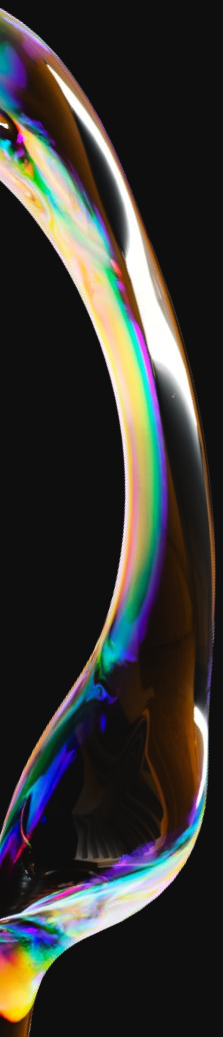
INDUCTIVA



Running Simulations at Scale Using Inductiva Python API

Presented by Luis Sarmento
CEO & Cofounder

sarmento@inductiva.ai



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What is **Inductiva?**

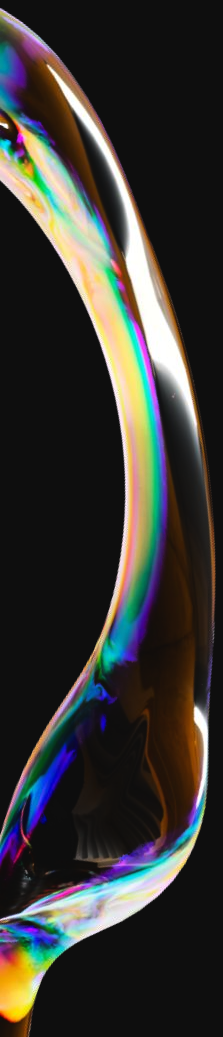
We're a startup born in 2021 to make large-scale simulations both accessible and affordable—**for everyone**.

Inductiva API is a cloud-based **High-Performance Computing (HPC) platform** designed to simplify and scale large-scale simulation workflows across various engineering and scientific domains.

Inductiva API

Key Features

- Wide Application Range
- Scalable Cloud Infrastructure
- Streamlined Workflow
- Easy Access



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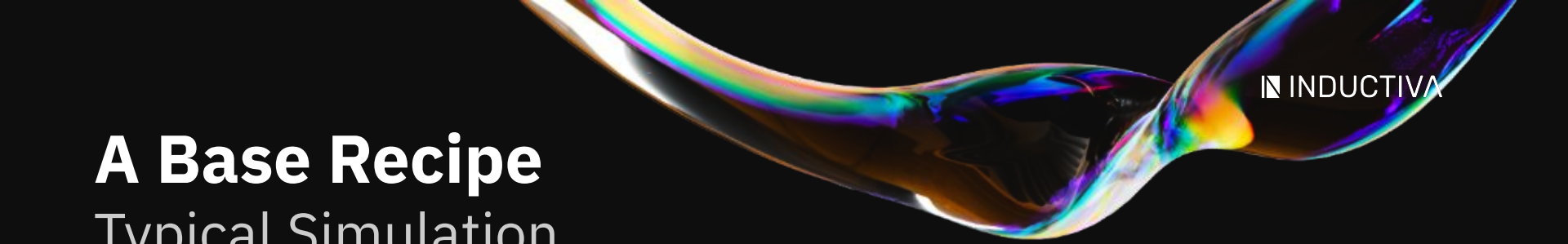
Why Python for Simulations?

We are not simply a Python-based API.

Python is more than a programming language, it is also **the language of AI**.

Python
Key Advantages

- Python’s Popularity
- Simple and Readable
- Perfect for Automating Workflows
- Huge Community and Support



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A Base Recipe

Typical Simulation Workflow

Prepare your Simulation Files → **Run Simulation** on your Local Machine → **Wait** for your Results → **Analyze** your Data

INDUCTIVA

A Base Recipe

Why Typical Simulation Workflows *Fall Short*?

- **Time Consuming**
- **Limited Scalability**
- **Resource Constraints**

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Inductiva's Base Recipe

The Inductiva-Supercharged Simulation Workflow

Prepare your Simulation Files → **Select** a Cloud Machine → **Free Up** Your Local Resources → **Analyze** your Data

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Inductiva's Base Recipe

The Inductiva-Supercharged Simulation Workflow

With Inductiva's workflow, **you no longer have to wait for simulations** to finish.

Run them efficiently in the background while staying productive on other tasks.

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A Closer Look

The Inductiva-Supercharged Simulation Workflow

Let’s break down each step of running a simulation with **Inductiva** and see how it transforms your typical workflow.

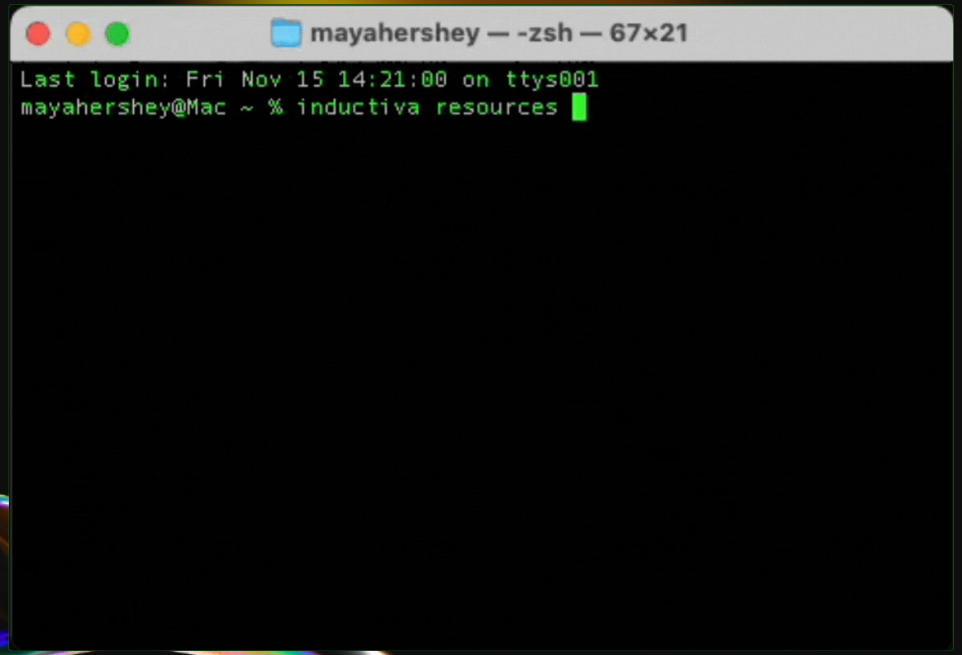
Pick a **Cloud Machine** → **Pick** Your **Simulator** → **Start** Your Simulation → **Stop** Your Machine & **Analyze** Results

INDUCTIVA

1. Pick a Cloud Machine

List Available Machines

The `inductiva resources available` command displays **a list of machines**, including their types, configurations, and capabilities.



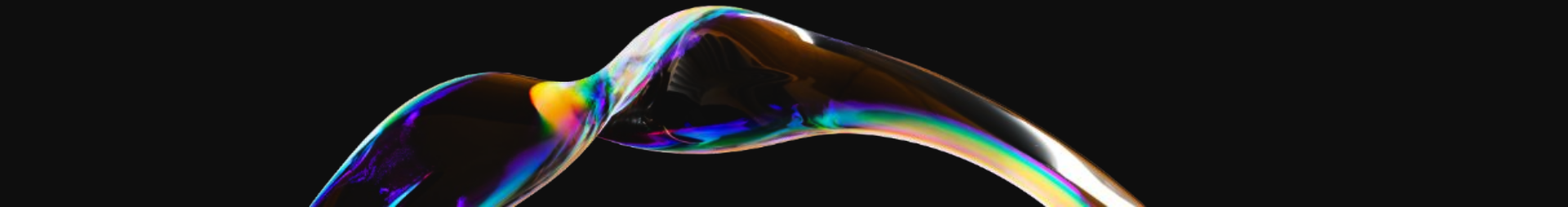
INDUCTIVA

1. Pick a Cloud Machine

List Available Machines

When selecting a machine, Inductiva **offers various configuration** options to optimize performance and costs.

- ➔ **Spot Instances**
- ➔ **Automatic Disk Resizing**
- ➔ **Maximum Idle Time**



INDUCTIVA

1. Pick a Cloud Machine

Configure and Start one Machine

After you've checked the available resources and selected a machine, here's how to configure and **start it.**

```
mg = inductiva.resources.MachineGroup(
    machine_type="c2d-highcpu-112",
    spot=True,
    data_disk_gb=20,
    auto_resize_disk_max_gb=100)
```

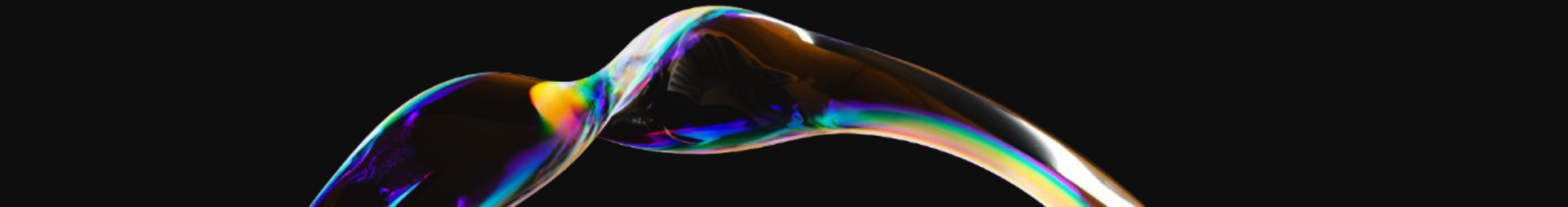
INDUCTIVA

1. Pick a Cloud Machine

Configure and Start Multiple Machines

Need to run multiple simulations in parallel? You can select and **start multiple machines.**

```
mg = inductiva.resources.MachineGroup(
    machine_type="c2d-highcpu-112",
    data_disk_gb=20,
    num_machines=5)
```



INDUCTIVA

2. Pick Your Simulator

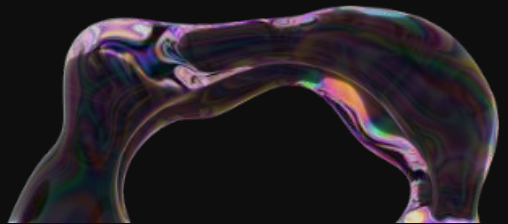
List Available Simulators

The `inductiva simulators ls` command lists the available simulators integrated into the Inductiva API, along with their supported versions.

```
AVAILABLE SIMULATORS AND VERSIONS FOR PRODUCTION RUNS:

SIMULATOR              VERSIONS
amr-wind               1.4.0
cans                   2.3.4
dualsphysics           5.2.1
fds                    6.8
fvcom                  5.1.0
gromacs                2022.2
nwchem                 7.2.2
openfast               3.5.2
openfoam-esi           2406, 2206
openfoam-foundation    8
quantum-espresso       7.3.1
reef3d                 24.02
schism                 5.11.0
splishsplash           2.13.0
swan                   41.45
swash                  10.01A, 10.05, 9.01A
xbeach                 1.24, 1.23

mayahershey@Mayas-MacBook-Air ~ %
```



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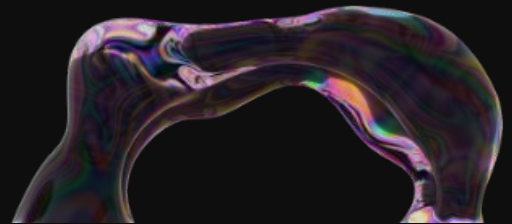
2. Pick Your Simulator

Choose a Simulator

Once you've identified the simulator you want to use, initialize it in your Python script. Let's pick Reef3D.

```
reef3d = inductiva.simulators.REEF3D()
```



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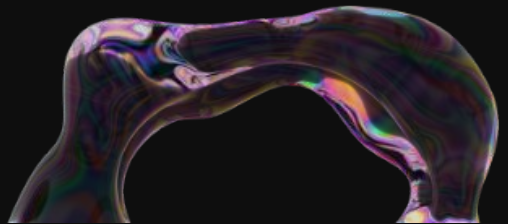
2. Pick Your Simulator

Specify a Simulator Version

Once you've selected your simulator, specify the version you want to use. Here's an example with the SWASH simulator.

```
swash                          10.01A, 10.05, 9.01A
```

```
swash = inductiva.simulators.SWASH(version="10.05")
```



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3. Start Your Simulation

Run the Simulation

Once your simulator and machine are set up, **start your simulation** on the configured machine, with all resources allocated as specified.

```
task.wait()
task.download_outputs()
machine_group.terminate()
```

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4. Stop Your Machine & Analyze Results

```
task.wait()
```
Waits for your simulation to end.

```
task.download_outputs()
```
Downloads your simulation results.

```
machine_group.terminate()
```
Terminates your machine.

Inductiva API
Advanced Applications

- **Run your own simulator** using your custom Docker image.
- Scale even further with **MPI Clusters**.
- **Run many variations of a simulation** in parallel to explore parameter spaces or optimize designs.
- **Generate high-quality datasets** to train Physics AI models.
- **Evaluate and select the best hardware** configuration for your simulation tasks via benchmarking.

Inductiva API

Web Console

The Inductiva Console is a web-based interface that gives you full visibility and control over your simulations.

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Inductiva Web Console

Machine Groups

View all active and idle **machine groups**.

Machine Groups

Active | Available

Name	Machine Type	Elastic	Type	# Machines	Disk Size	Spot	Started At	Idle Time	Max Cost (per hour)
api-2atg26686omtskzp4qrsgpzgy	c2-standard-8	No	standard	2/2	10 GB	Yes	07/11/24, 09:21:46	00:02:01/00:30:00	0.26991555558 USD
api-6exu9z1zp03c7a53wf6w97d6f	c2-standard-8	No	mpi	2/2	10 GB	No	07/11/24, 09:22:27	00:01:19/00:30:00	0.94935555558 USD
api-i3ep6obi0t5ervuf5010eik9w	c2-standard-4	No	standard	1/1	10 GB	Yes	07/11/24, 09:20:46	00:03:01/00:30:00	0.07511777779 USD

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Inductiva Web Console

Simulation Tasks

View all active, completed, and queued **simulations.**

Simulation Tasks

Showing the 50 most recent tasks

Task Id ↑↓	Status ↑↓	Submit time ↑↓	Started ↑↓	Duration ↑↓	Simulator ↑↓	Project ↑↓	Estimated cost
q1vg8i60iq46izebdjs2qaazw	success	21/10/2024, 16:01:10	21/10/2024, 16:01:23	6 seconds	amrwind	pbarbosad6ca8462	0.0001 US$
hzbwk5xxry8pfxetjnyc9yfav	success	17/10/2024, 09:33:35	17/10/2024, 09:33:35	3 minutes, 48 seconds	openfoam_foundation	pbarbosad6ca8462	0.0038 US$
dji1nu1jefecwsmc71ec0xtdx	success	03/10/2024, 16:12:59	03/10/2024, 16:12:59	24 seconds	reef3d	pbarbosad6ca8462	0.0002 US$

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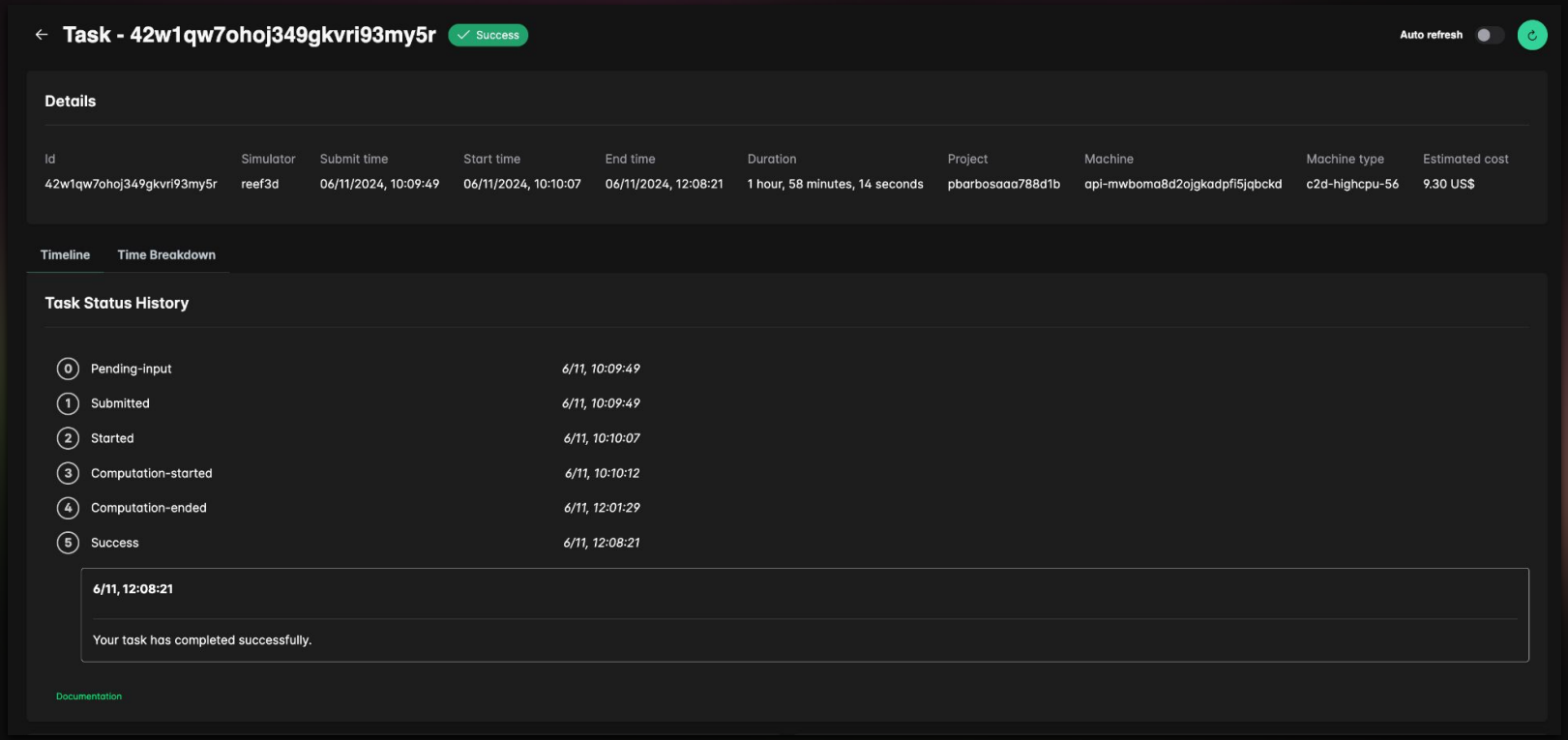
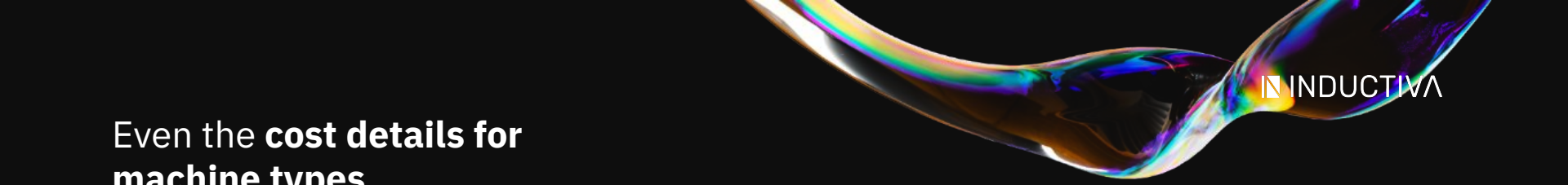
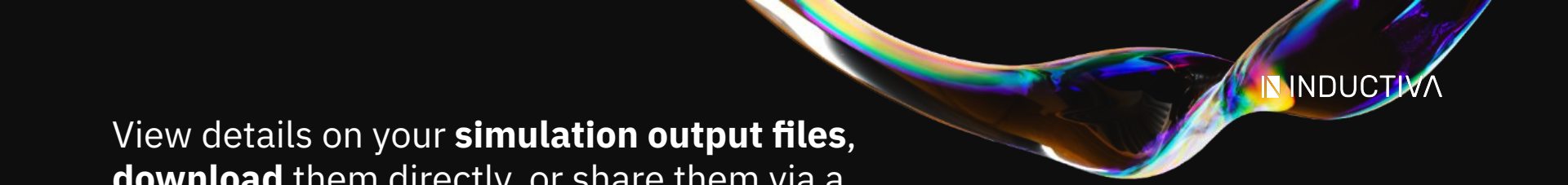
Or drill down into the **details of any simulation job**.





Even the **cost details for machine types.**

Machine type	Estimated cost
c2d-highcpu-56	9.30 US$



View details on your **simulation output files**, **download** them directly, or share them via a **shareable link**.

Output

Size zipped	Size unzipped	Number of files
12.40 GB	29.95 GB	142626

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View details on your **simulation logs,** from progress updates to error details.

stdout.txt stderr.txt

```
# COMMAND: ['/DIVEMesh/bin/DiveMESH']


DIVEMesh (c) 2008-2024 Hans Bihs

:: Open-Source Meshing


v_240216

read control
DXM: 0.025
xma:3 yma: 3 zma: 3
xmin:0 ymin: 0 zmin: 0
xmax:2 ymax: 1 zmax: 1
knox:80 knoy: 40 knoz: 40
base_cellnum3D: 128000
base_cellnum2D: 3200
field: 181976
slice: 3956

grid_spacing: DR: 0.025 DS: 0.025 DT: 0.025
```

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Inductiva Web Console

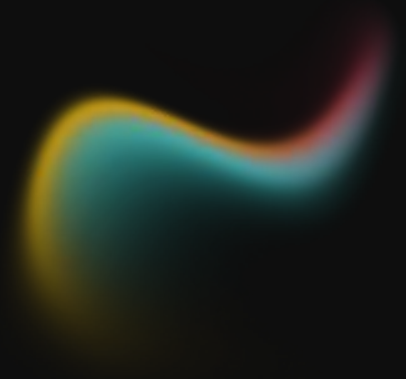
MOHID (Experimental)

```
cloud_machine = inductiva.resources.MachineGroup( \
   provider="GCP",
   machine_type="c3d-standard-180",
   spot=True)

# Initialize the MOHID
mohid = inductiva.simulators.MOHID()

# Run simulation
task = mohid.run(
   input_dir=”dir_with_artifacts”,
   working_dir="Level1/exe",
   command="MohidWater.exe",
   run_ddc=True,
   n_vcpus=180,
   on=cloud_machine)

task.wait()
```



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Inductiva API

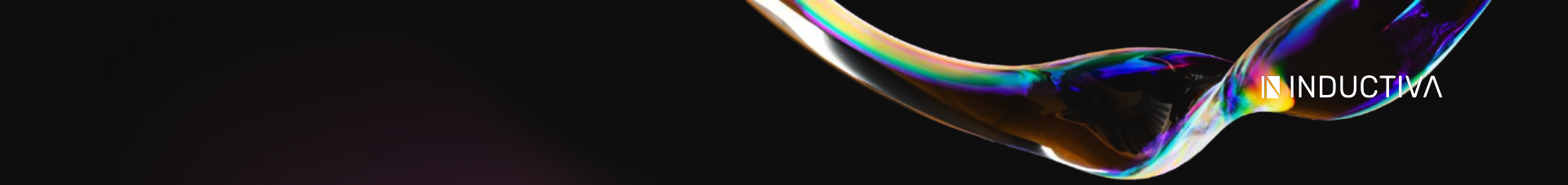
Getting Started

Before diving into the practical session and trying out the API together, we've prepared a simple onboarding process to help you set up everything you need.

Inductiva API
Pre-Requisites

To maximize hands-on time, we shared a **Prerequisite Guide** ahead of the session.

- Install Python and pip on your laptops.
- Ensure your environment is set up



Inductiva API
Onboarding Overview

With just these **three steps**, you'll be ready to explore the Inductiva API and start running your simulations. Here's what our onboarding process looks like:

1. **Register** and **Get Your API Key**
2. **Install** the Inductiva Python Package
3. **Authenticate** Your API Key

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Let’s Get Started!

Part 1: Create an Account

1. Go to: https://inductiva.ai/

2. Choose “Log In” (New Account)
Use your Gmail Account or type in your email.

3. After creating your account, you will be shown further installation instructions via Inductiva web console

Let’s go to Part 2.

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Let’s Get Started!

Part 2. Installing Inductiva Python client:

0. Make sure you have Python installed on your computer

1. From your command line terminal (Windows/OSX), do:

```
pip install inductiva
```

3. You now have Inductiva Python Client installed in your machine. In your terminal, type:

```
inductiva
```

You should see a few Inductiva command options.

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Let’s Get Started!

Part 3. Authenticate and Go!

1. From your command line terminal (Windows/OSX), do:

```
inductiva auth login
```

2. Copy paste your personal API Key you can see in the Console, and press Enter.

3. Choose one of the examples that were automatically downloaded. E.g.

```
python inductiva_examples/openfoam_esi.py
```

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Thank You!