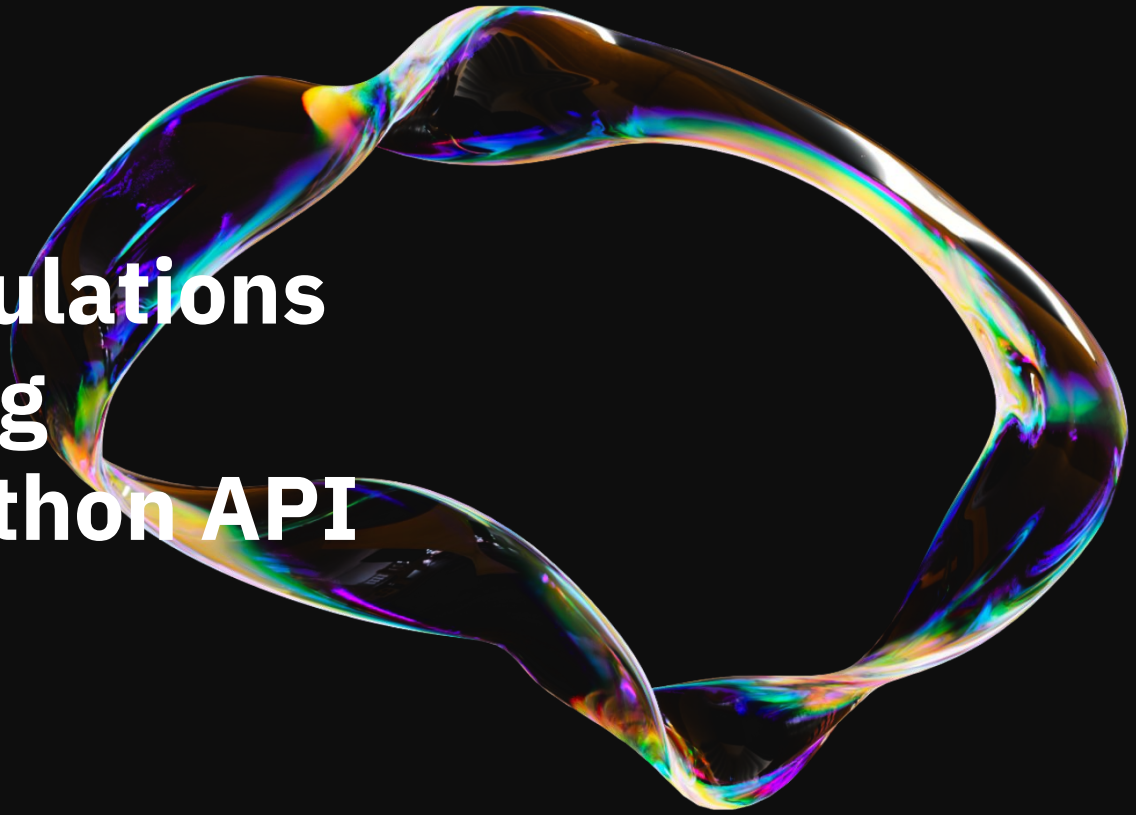
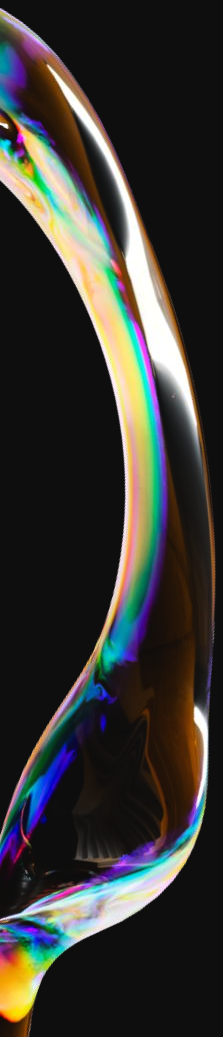
INDUCTIVA



Running Simulations at Scale Using Inductiva Python API

Presented by Paulo Barbosa
Software Engineer - Inductiva

pbarbosa@inductiva.ai

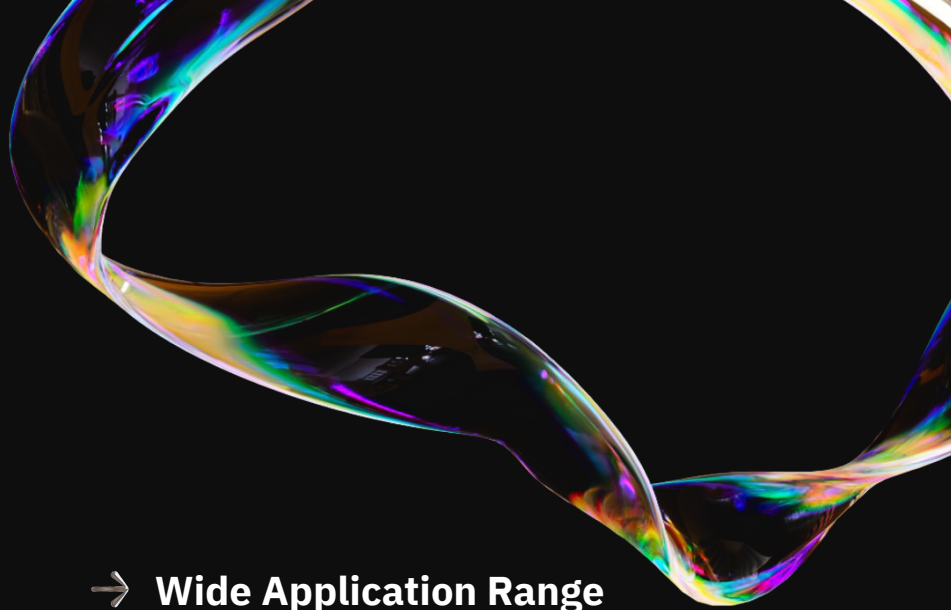


INDUCTIVA

What is **Inductiva?**

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

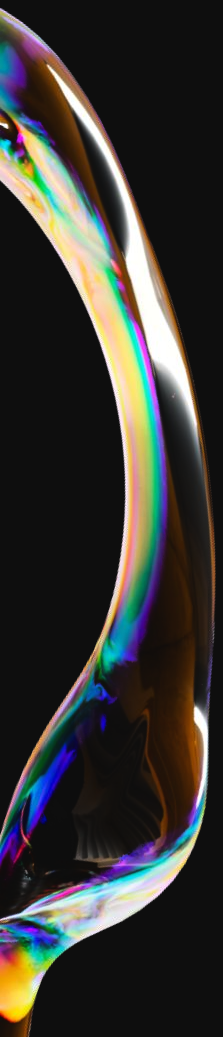
Inductiva API is a cloud-based **High-Performance Computing (HPC) platform** designed to simplify and scale large-scale simulation workflows across various engineering and scientific domains.



Inductiva API

Key Features

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



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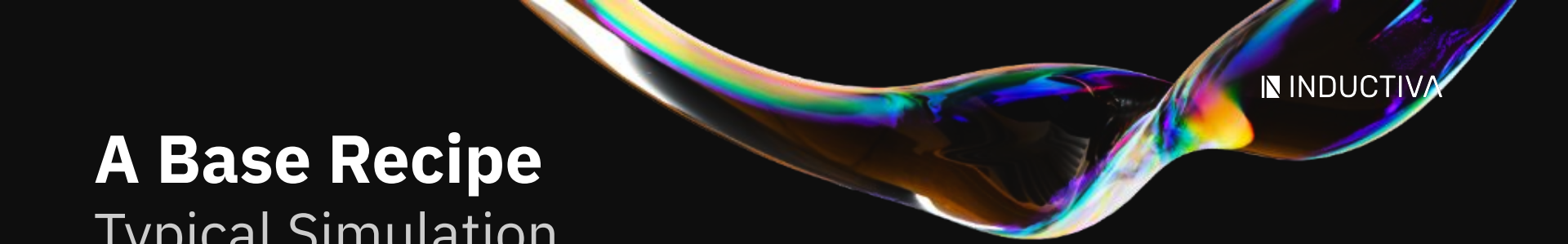
Why Python for Simulations?

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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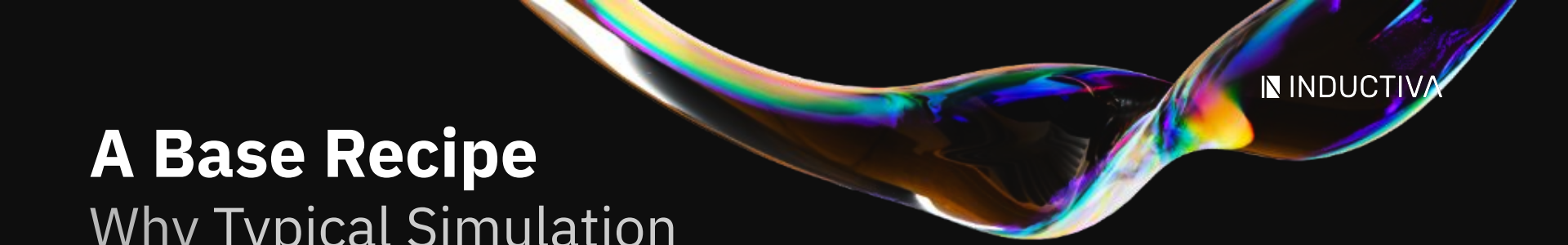
A Base Recipe

Typical Simulation Workflow

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



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A Base Recipe

Why Typical Simulation Workflows *Fall Short*?

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

INDUCTIVA

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.

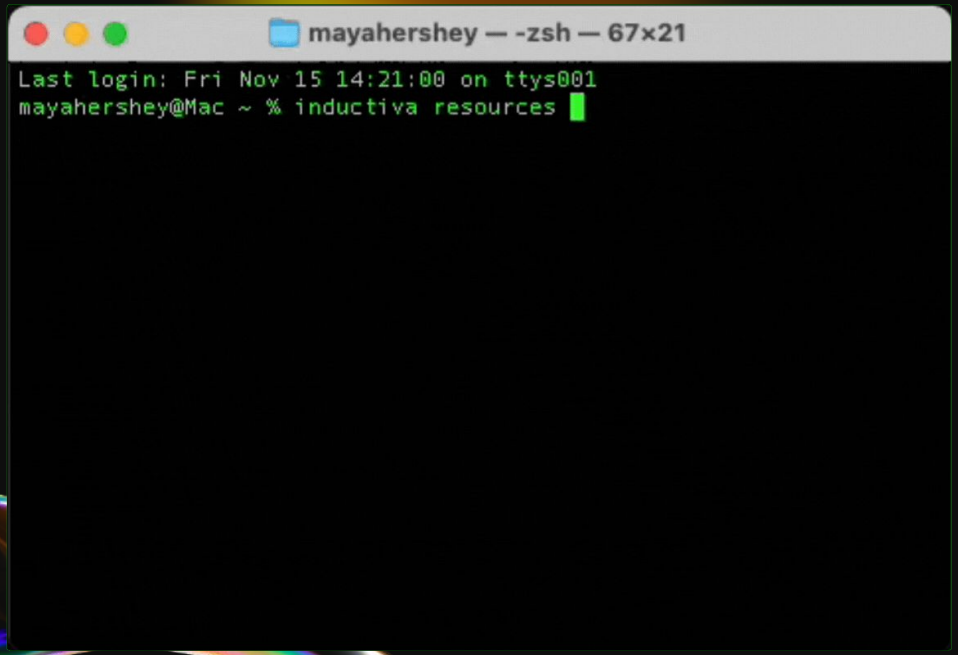
Pick a **Cloud Machine** → **Pick** Your **Simulator** → **Start** Your Simulation → **Stop** Your Machine & **Analyze** Results

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.



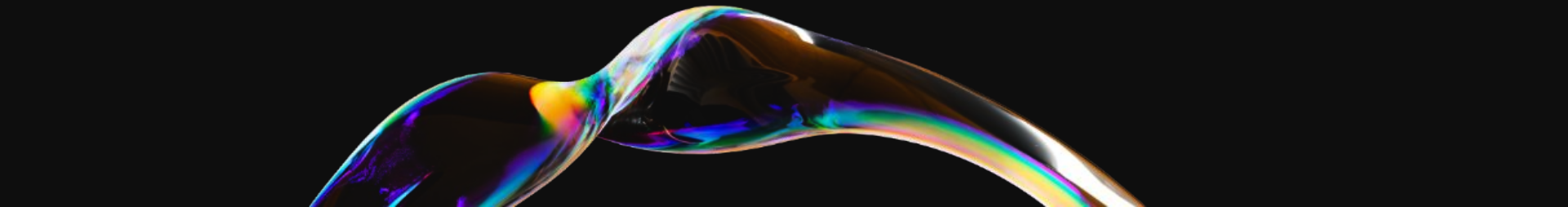
INDUCTIVA

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**



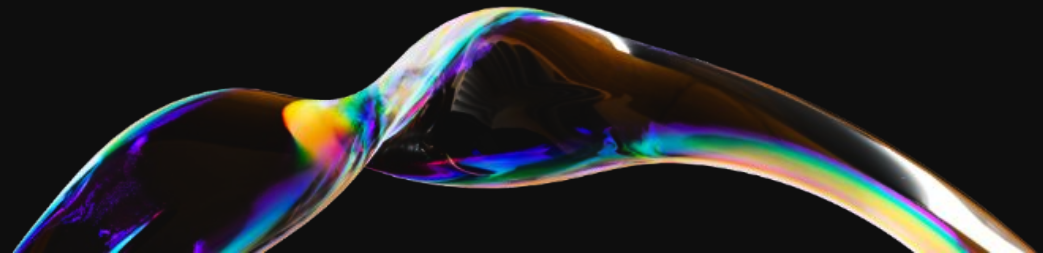
INDUCTIVA

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,
    max_idle_time=
        datetime.timedelta(minutes=1))
mg.start()
```



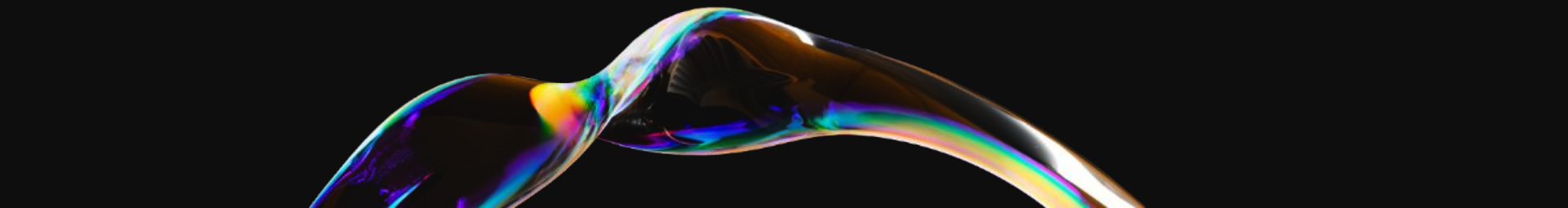
INDUCTIVA

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)
mg.start()
```

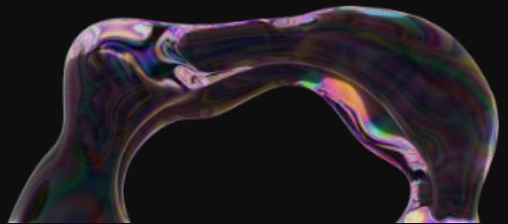


INDUCTIVA

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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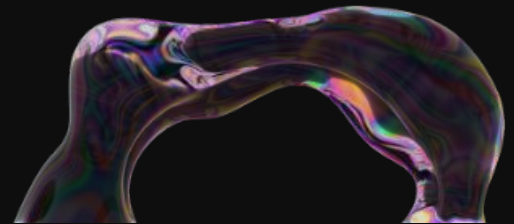
2. Pick Your Simulator

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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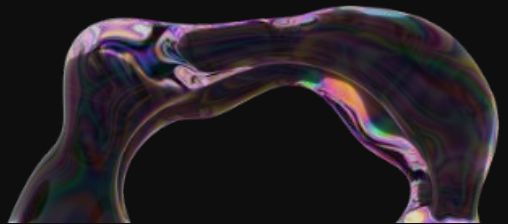
2. Pick Your Simulator

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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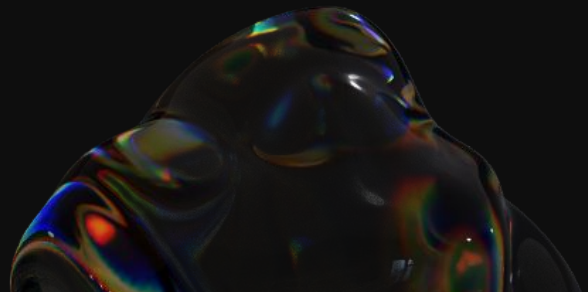
3. Start Your Simulation

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 = reef3d.run(
    input_dir=input_dir,
    on=machine_group,
    n_vcpus=56,
    use_hwthread=False,
    storage_dir="3D_dam_break_with_obstac
le")
```



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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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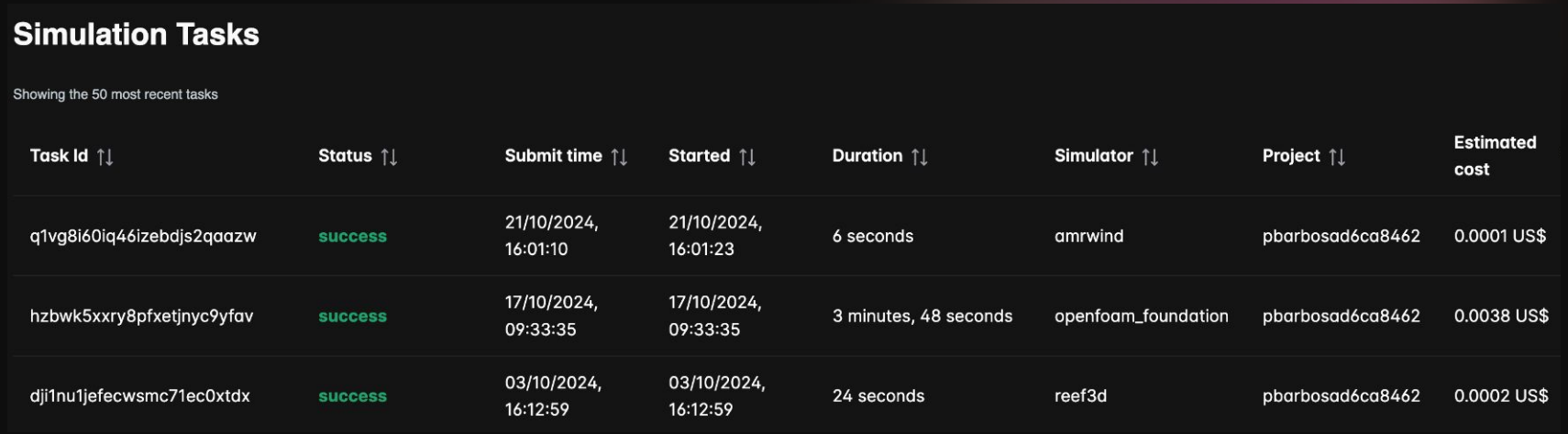
Inductiva Web Console

Simulation Tasks

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



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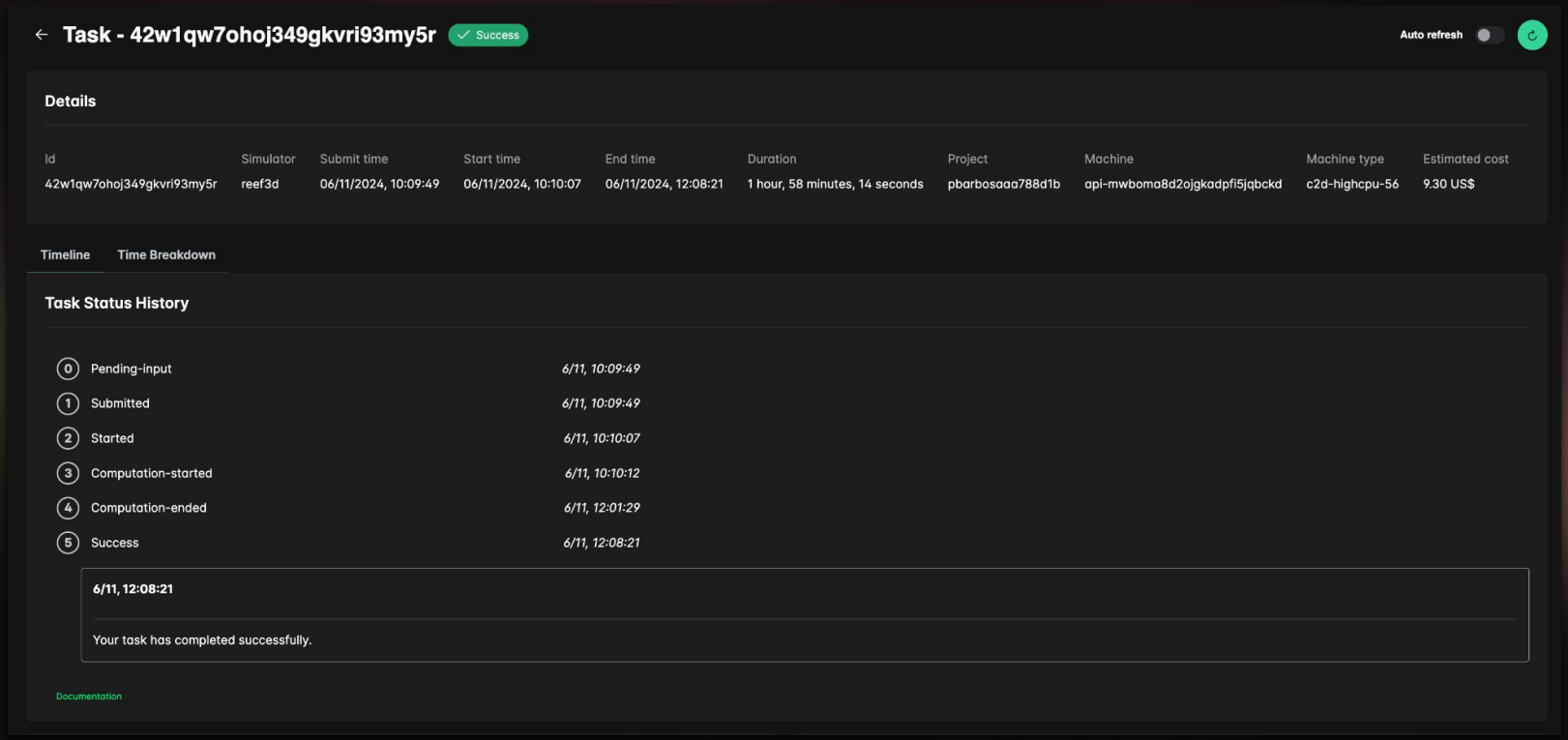
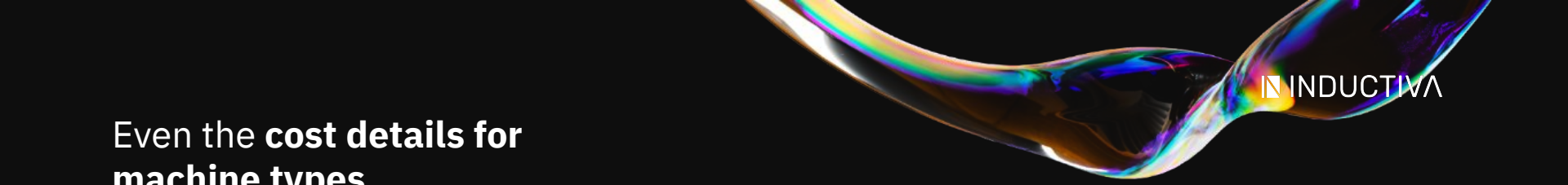
Or drill down into the **details of any simulation job**.





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

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

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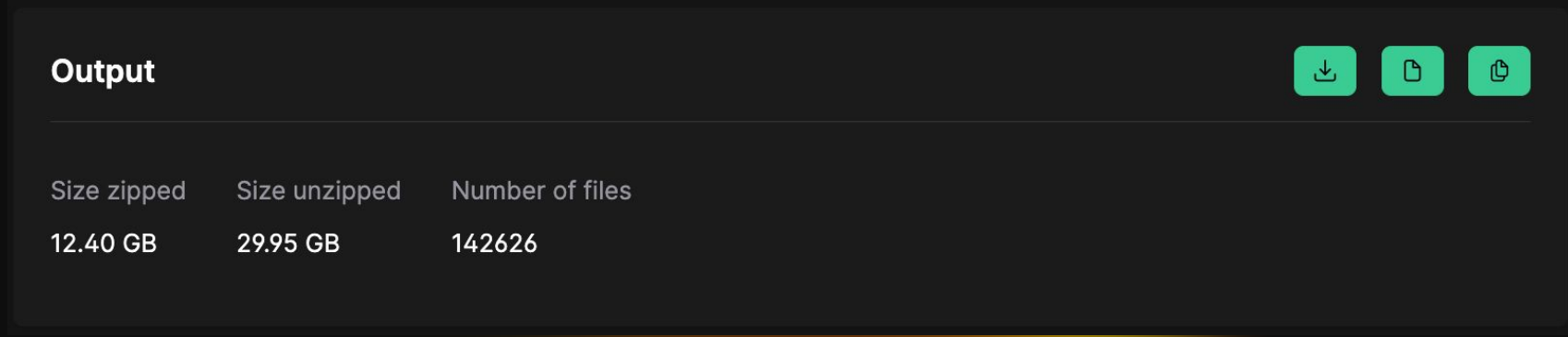
View details on your **simulation output files**, **download** them directly, or share them via a **shareable link**.



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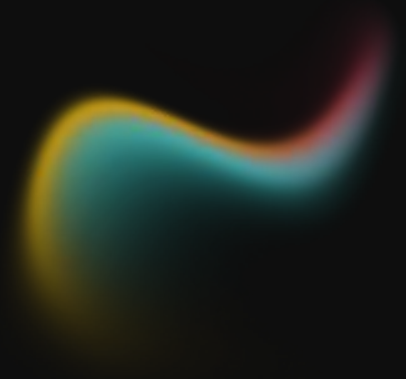
View details on your **simulation logs,** from progress updates to error details.

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 API

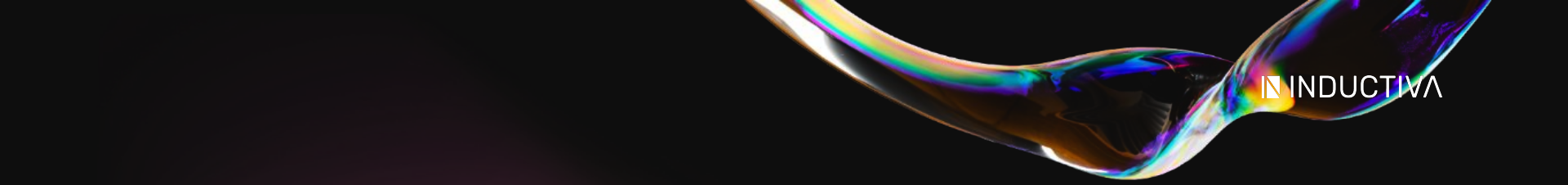
Getting Started

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!

Coming up next:

Join Us in Our Tutorial

- ➔ Get hands-on experience with the Inductiva API.
- ➔ Set up your environment and run a simulation on the cloud.

Explore Advanced Applications (*if time allows*)

Dive deeper into advanced capabilities like custom simulators, MPI clusters, or dataset generation.

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Thank You!

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