



# OpenFOAM meeting

## 1. VS code remote

```
File Edit Selection View Go Debug ... dataGen.py - neuralODE_combustion [SSH: gpu133] - Visua...  
REMOTE-SSH  
CONNECTIONS  
  gpu133  
    neuralODE_combustion /home/edis...  
    LRT10Foam /home/edison/repos  
  gpu134  
    LRT10Foam /home/edison/repos  
    gcp  
FORWARDED PORTS  
No ports are being forwarded from "gpu133".  
Forward a port.  
HELP AND FEEDBACK  
  ★ Getting Started  
  📖 Read Documentation  
  🐦 Provide Feedback  
  ⓘ Review Issues  
  💬 Report Issue  
src ▾ dataGen.py  
132 dask.config.set(scheduler='processes')  
133  
134 s = time.time()  
135 You, a month ago · add neuralode  
136 a = [delayed(ignite_f)(x[0], x[1], 'H2')  
137 a = dask.compute(*a)  
138  
139 print('a[0][0]={}'.format(len(a[0][0])))  
140 e = time.time()  
TERMINAL 1: bash  
edison@Node133:~/repos/neuralODE_combustion$ ls  
base_neuralODE.h5  img  README.md  
boost_test.py  input_preprocessing.py  rk4Model.h5  
chem_test  LICENSE  savedModel  
clustering.py  neuralODE_post.py  src  
data  neuralODE_train.py  stiffODE.py  
delta_res_nets.py  notebooks  tf2.py  
distributed.py  pb2uff  tmp  
draft.md  pca_filter.py  tmp.png  
fig  postODENet.h5  wudi.h5  
edison@Node133:~/repos/neuralODE_combustion$
```

## 2. Dask



# DASK

Dask natively scales Python

Dask provides advanced parallelism for analytics, enabling performance at scale for  
the tools you love

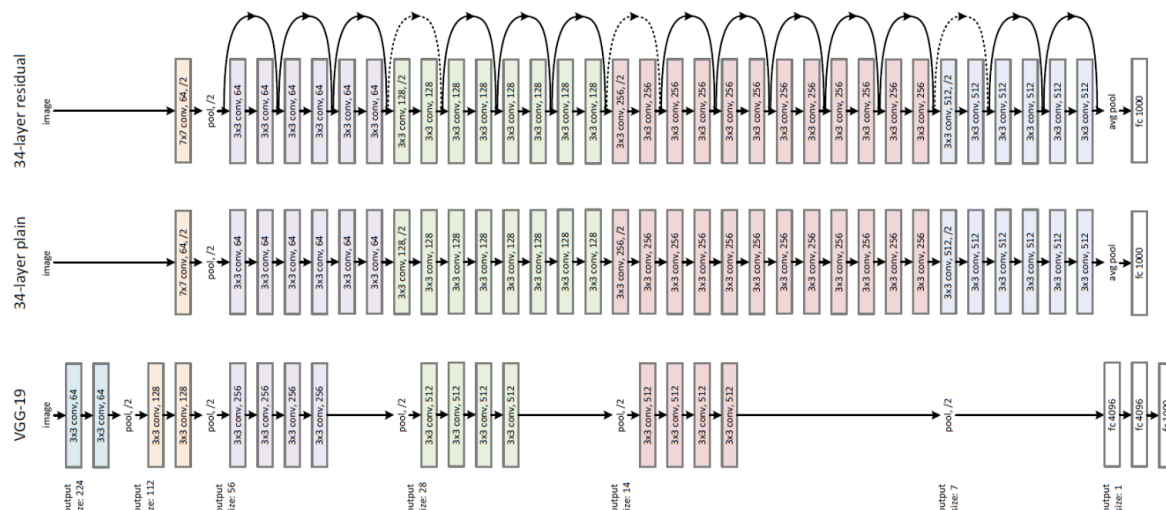


### 3. Neural ODE for chemical reactions

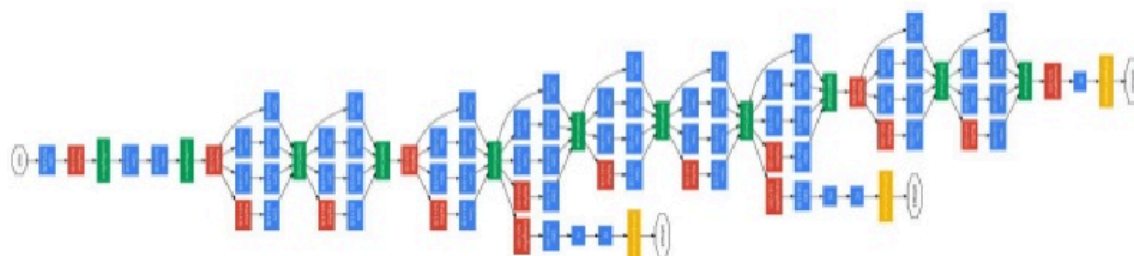
- MLP

mlp

- Deep Neural Networks



GoogleNet or Inception (2014)



- Neural ODE

## Computer Science &gt; Machine Learning

# Neural Ordinary Differential Equations

Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, David Duvenaud

*(Submitted on 19 Jun 2018 (v1), last revised 15 Jan 2019 (this version, v4))*

We introduce a new family of deep neural network models. Instead of specifying a discrete sequence of hidden layers, we parameterize the derivative of the hidden state using a neural network. The output of the network is computed using a black-box differential equation solver. These continuous-depth models have constant memory cost, adapt their evaluation strategy to each input, and can explicitly trade numerical precision for speed. We demonstrate these properties in continuous-depth residual networks and continuous-time latent variable models. We also construct continuous normalizing flows, a generative model that can train by maximum likelihood, without partitioning or ordering the data dimensions. For training, we show how to scalably backpropagate through any ODE solver, without access to its internal operations. This allows end-to-end training of ODEs within larger models.

Subjects: **Machine Learning (cs.LG)**; Artificial Intelligence (cs.AI); Machine Learning (stat.ML)Cite as: **arXiv:1806.07366 [cs.LG]**(or **arXiv:1806.07366v4 [cs.LG]** for this version)

- **Runge kutta network**

## Runge kutta 4th order method

$$k_1 = hf(x_n, y_n)$$

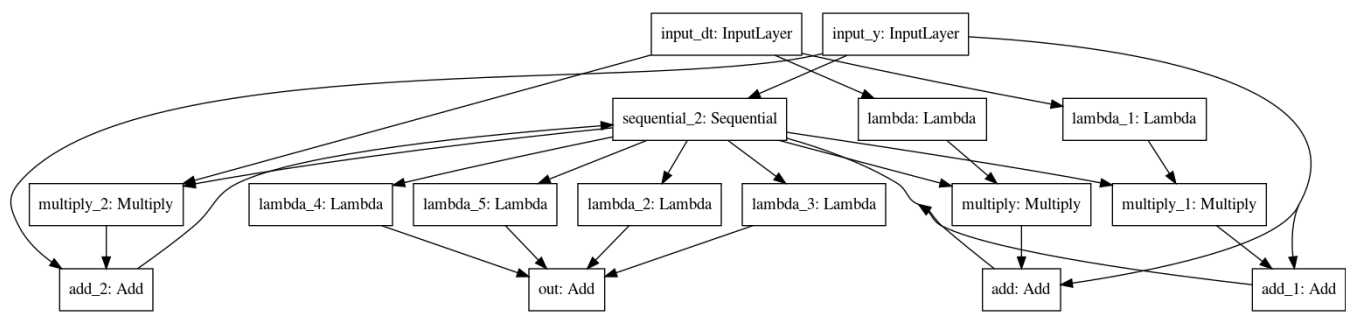
$$k_2 = hf(x_n + h/2, y_n + k_1/2)$$

$$k_3 = hf(x_n + h/2, y_n + k_2/2)$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

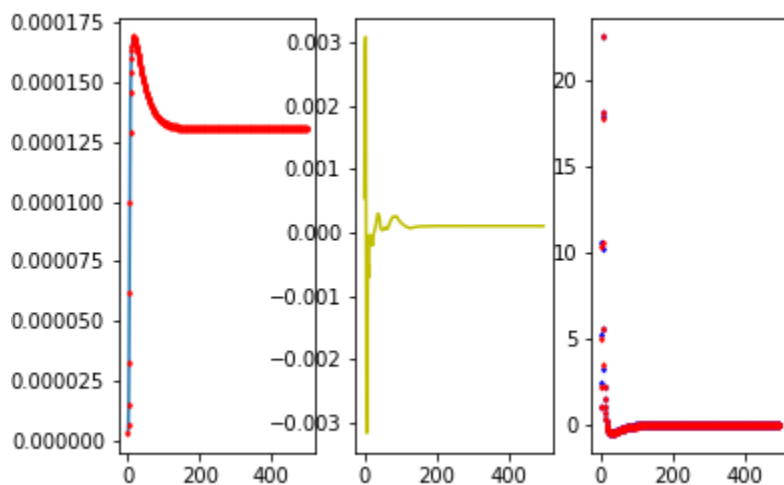
$$y_{n+1} = y_n + 1/6(k_1 + 2k_2 + 2k_3 + k_4)$$

## RK45Network

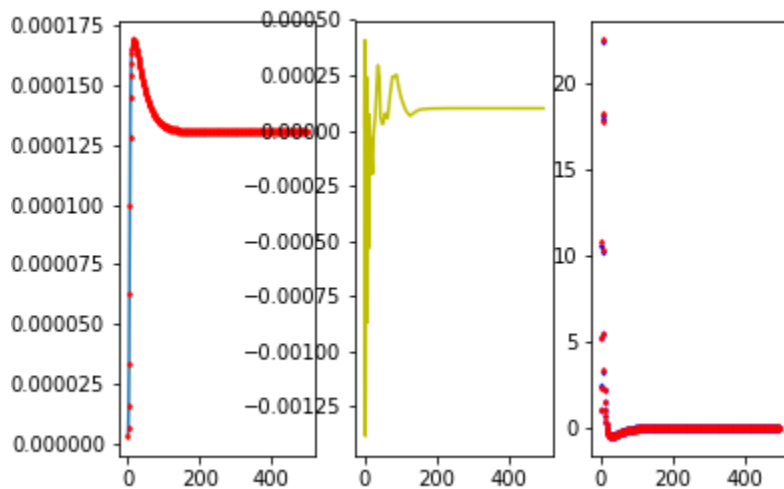


## H2 auto ignition

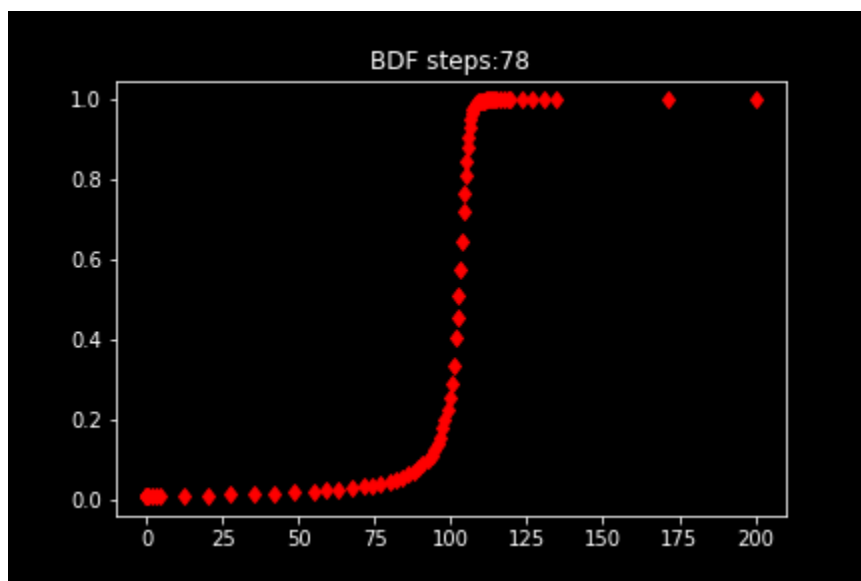
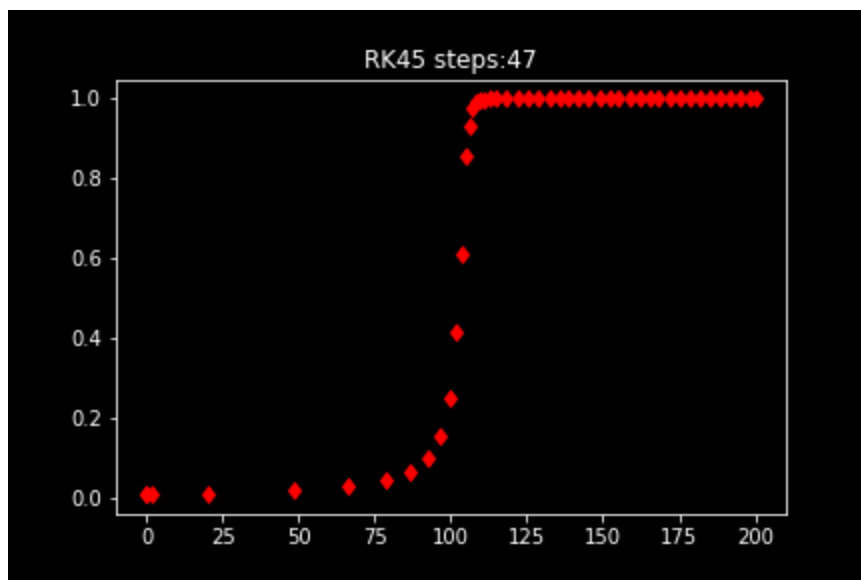
EULER: OH, T=1401

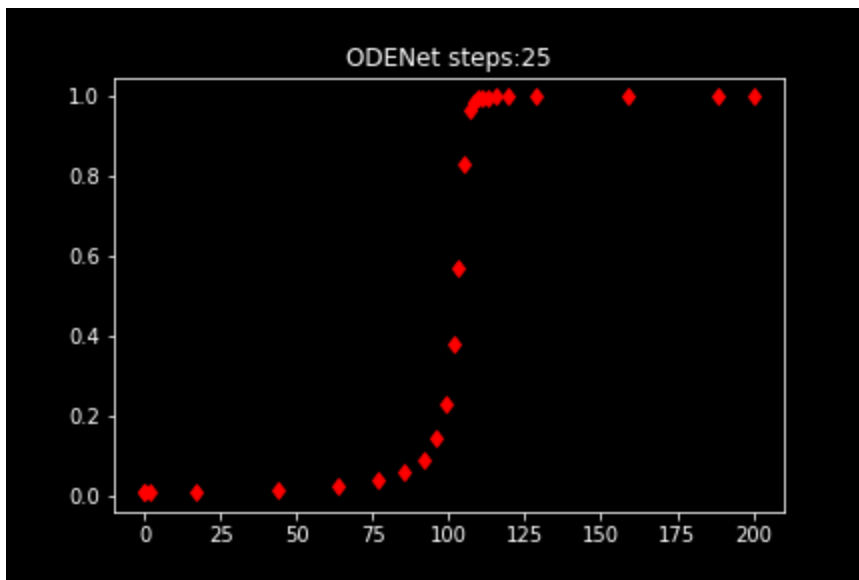


RK4: OH, T=1401



- explicit or implicit  
flame expansion





## Star me on github

**Overview** Repositories 16 Projects 0 Stars 21 Followers 8 Following 5

**Popular repositories**

- combustionML**  
a repo for adopting machine learning in combustion simulation  
Jupyter Notebook ★ 11 V 2
- neuralODE\_combustion**  
neural ode applied in combustion modelling  
Jupyter Notebook ★ 2
- ember**  
Forked from spethember  
Quasi-1D Unsteady Flame Solver  
C++
- oftft**  
Integrate neural network inference into OpenFOAM  
C++ ★ 3 V 2
- gltf\_react**  
JavaScript ★ 1
- cantera**  
calculating reaction rate in cantera  
Jupyter Notebook

**164 contributions in the last year**

Contribution activity

2019

June 2019

2018

[https://github.com/uqyge/neuralODE\\_combustion](https://github.com/uqyge/neuralODE_combustion)