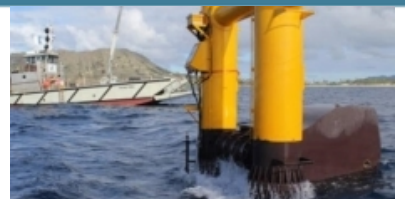
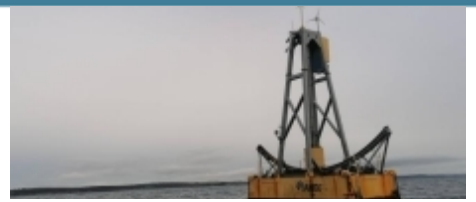
SAND2023-07612C

Sandia National Laboratories

Cornell University

Differentiable programming to enable modern optimization methods for MRE





Carlos A. Michelén Ströfer (Sandia)

Dr. Maha Haji & Kapil Khanal (Cornell)

U.S. DEPARTMENT OF ENERGY NNSA

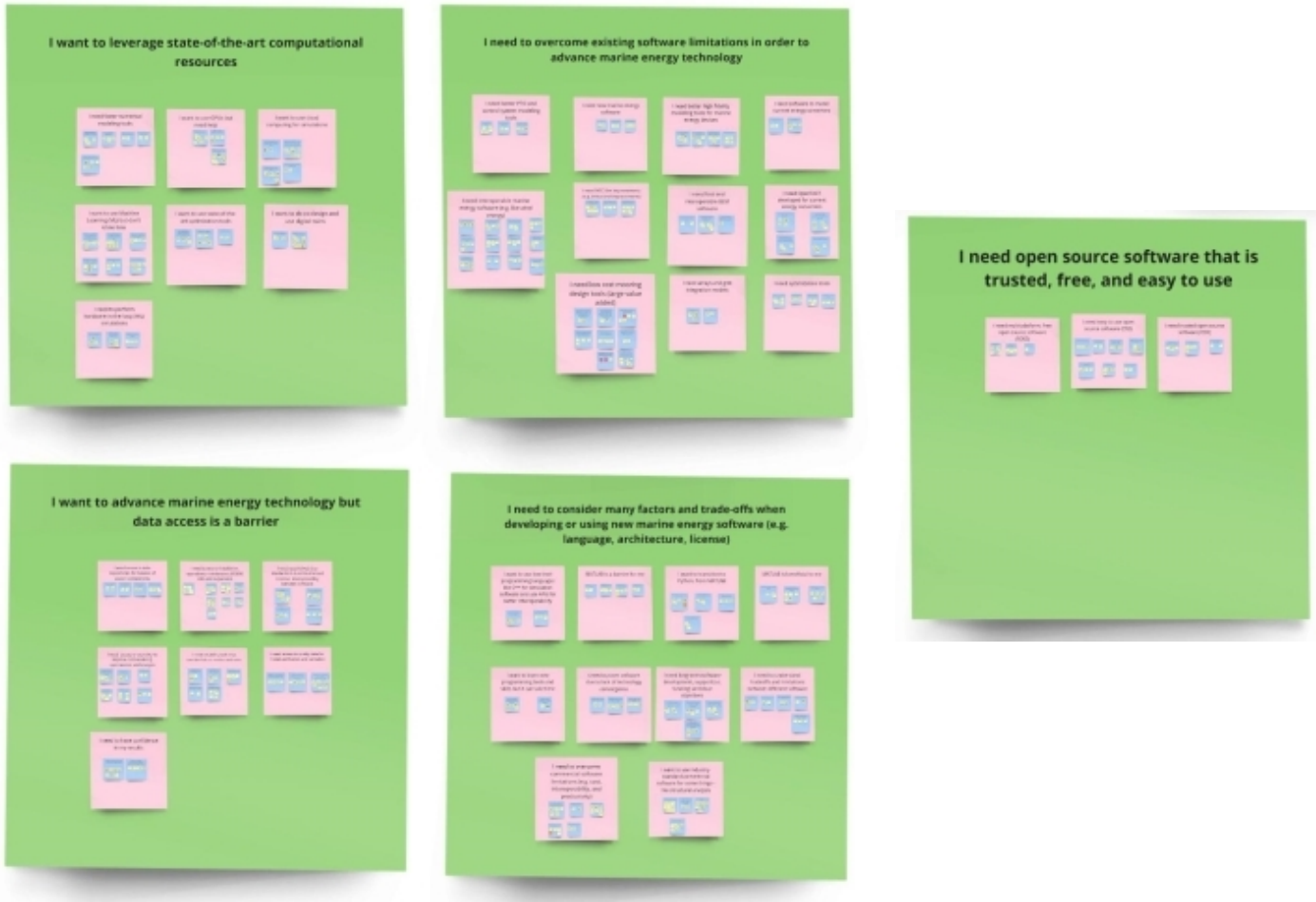
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Overview

- Scientific computing is hugely different today as compared to even five years ago in both the software and hardware landscapes.
- The amazing advances delivered by these methods are dependent on a critical technology: *differentiable programming*.
- ***We propose creating a differentiable and portable boundary element method (BEM) solver*** that will allow for modern and complex workflows in the design and optimization of wave energy converters (WECs).
- *Differentiability* will enable the use of novel methods such as adjoint-based multi-disciplinary optimization and data-driven methods such as physics-informed machine learning.
- *Portability* will make high-performance computing more accessible to everyday users through cloud computing and allow running the same code in different architectures such as GPUs.
- If successful, the project is expected to lead to completely new methods in the design of marine renewable energy.

Next-Gen Software needs & gaps assessment




I want to leverage state-of-the-art computational resources
I need faster numerical modeling tools
I want to use GPUs but need help
I want to use cloud computing for simulations
I want to use Machine Learning (ML) but don't know how
I want to use state-of-the-art optimization tools
I want to do co-design and use digital twins
I need to perform hardware-in-the-loop (HIL) simulations

Automatic Differentiation

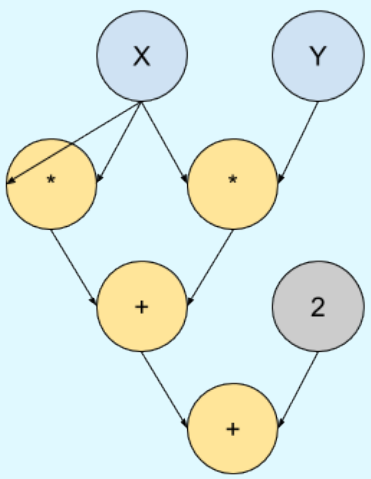
Finite difference

- cost = n_inputs * function

$$f' = \frac{f(x+h)-f(x)}{h}$$

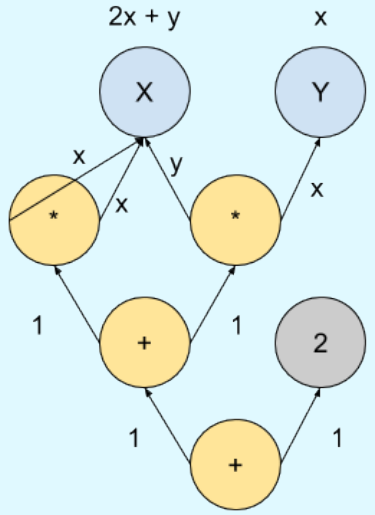
Automatic differentiation

- cost = 2 * function



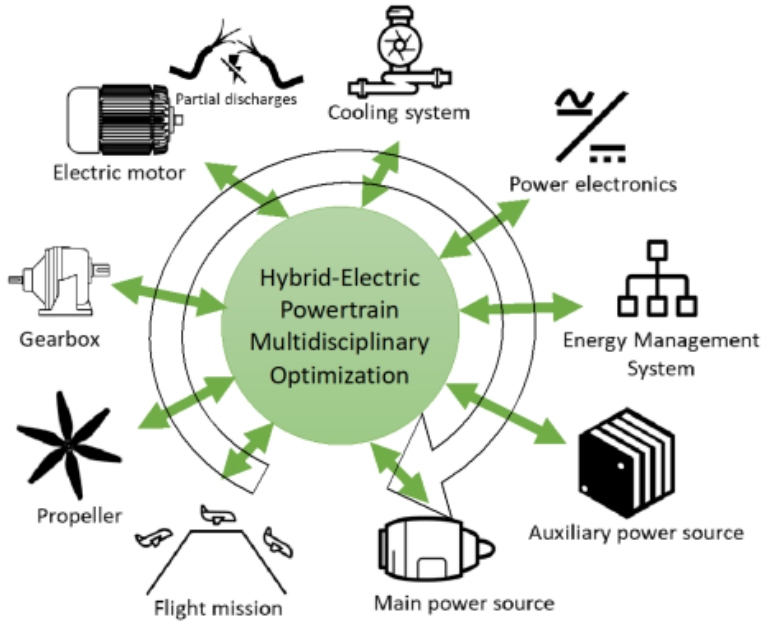
Computational Graph

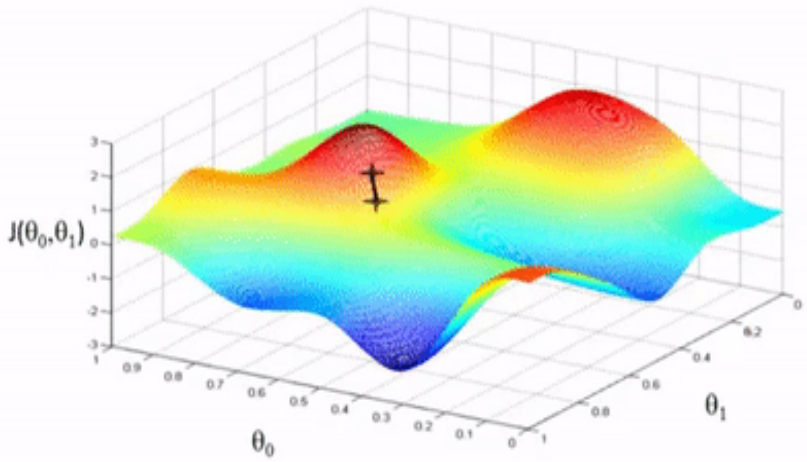
$x^2 + xy + 2$

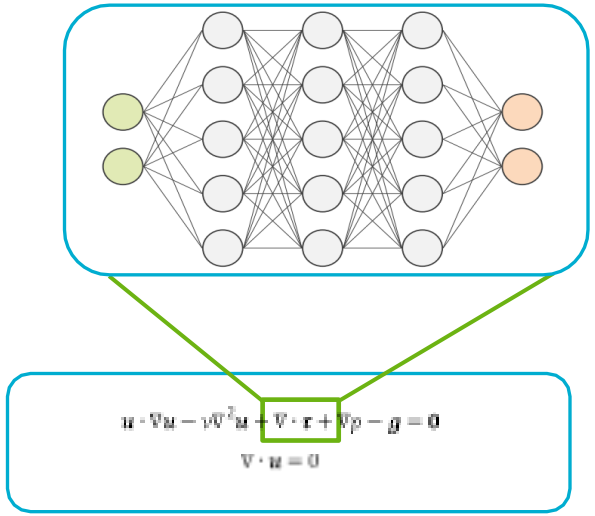


Backpropagation

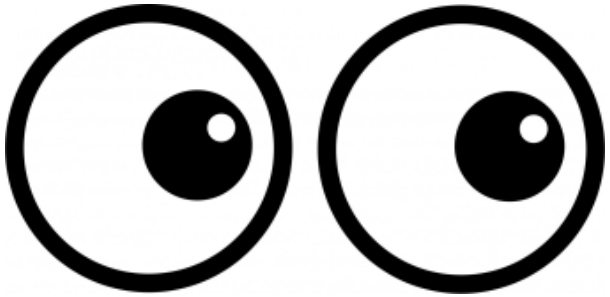
- **Why do we need the gradients?**
  - Adjoint-based optimization
    - Large multi-disciplinary optimization
    - Non-parametric geometry optimization
  - Control co-design
  - Physics-informed machine learning

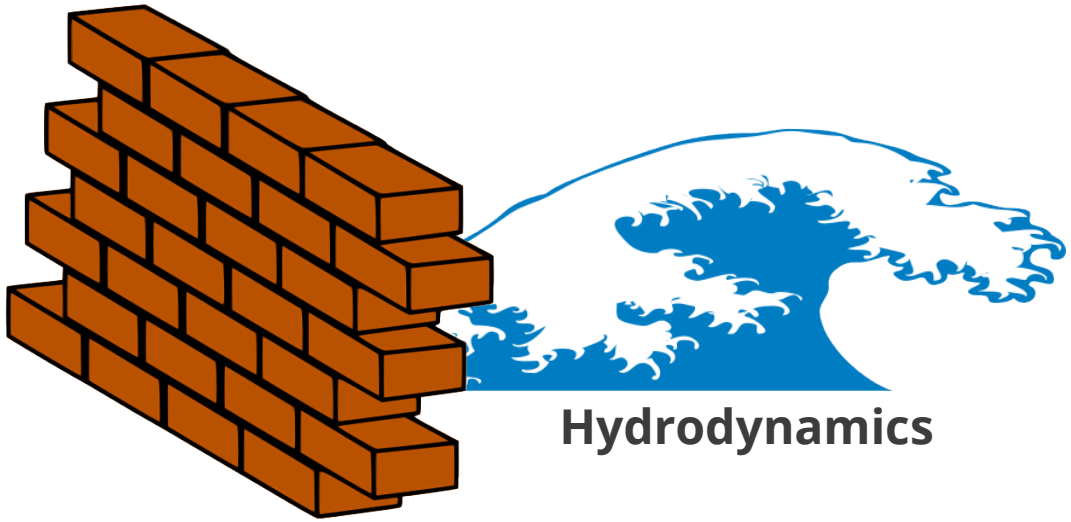






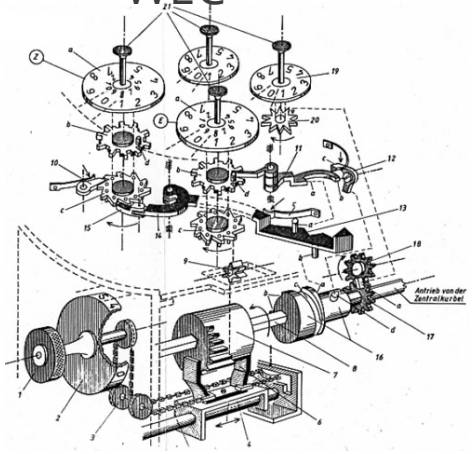
Current options don't allow automatic differentiation to *see* hydrodynamics





Hydrodynamics

WEC



Power take-off (PTO)

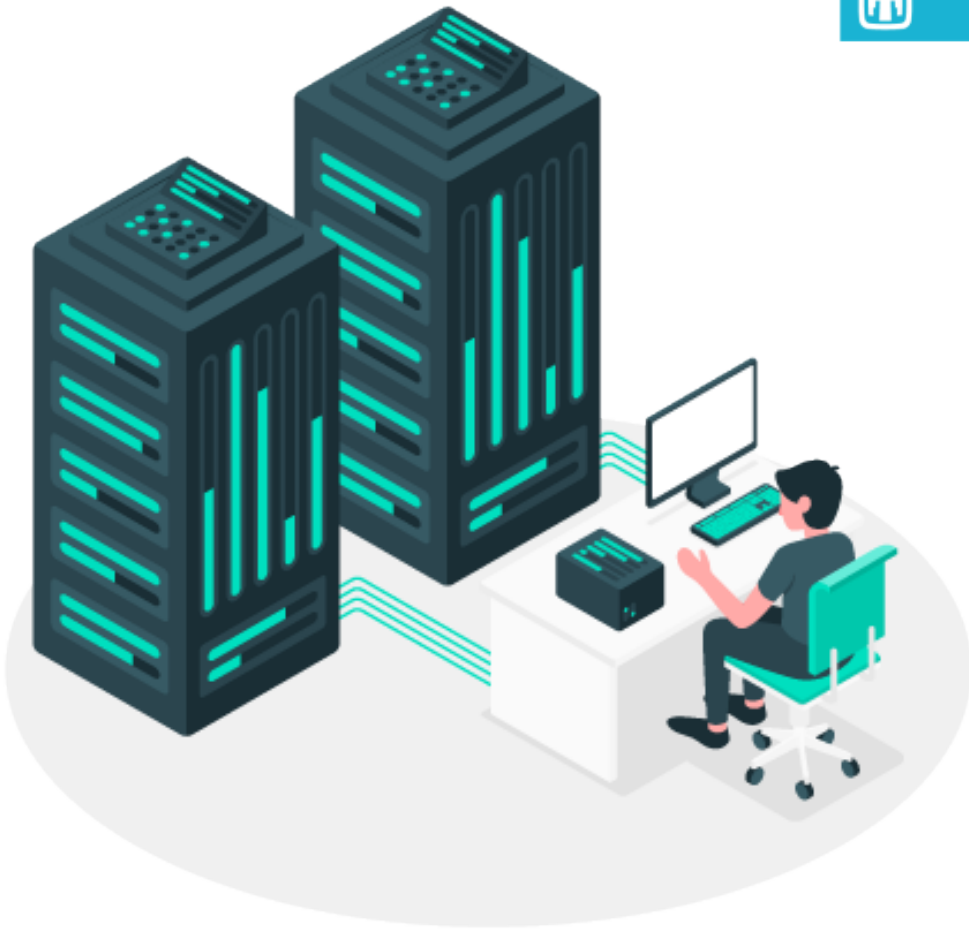
PEARL

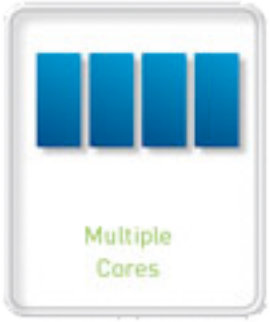
Propulsion
power management
satellite communications

Portability

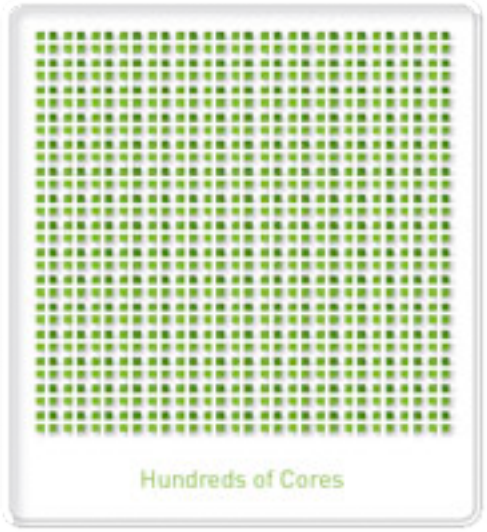
Same code should run in

- Personal computer
- HPC
- GPUs
- Cloud-computing





CPU
Serial tasks



GPU
Parallel

Julia

- Two-language problem
- Open source like Python, scientific computing like Matlab
- Large state-of-the art scientific computing, scientific machine learning, and optimization
- Differentiability
- Portability

Examples

- ARPA-E offshore floating wind project: MDO, differentiability
- NASA Recursat project: 15,000x speedup, PIML

Current status

- Contract with Cornell & bi-weekly meeting
- Literature review and understand different solution methods for the Greens function
- Selection of *Wu et al.* method for speed, simplicity, and ability to parallelize.
- Exploration of using splines for geometries and higher order methods for discretization.
- Initial implementation of *Wu et al.* in Julia.

Summary

- Differentiable code would enable adjoint-based multi-disciplinary optimization, advance ML, etc.
- A modern code should be portable, able to run in serial on a personal computer or parallel in a GPU cluster.
- This project is a proof of concept differentiable and portable BEM code.
- BEM is a major road block on several projects currently trying to use automatic differentiation.

cmichel@sandia.gov