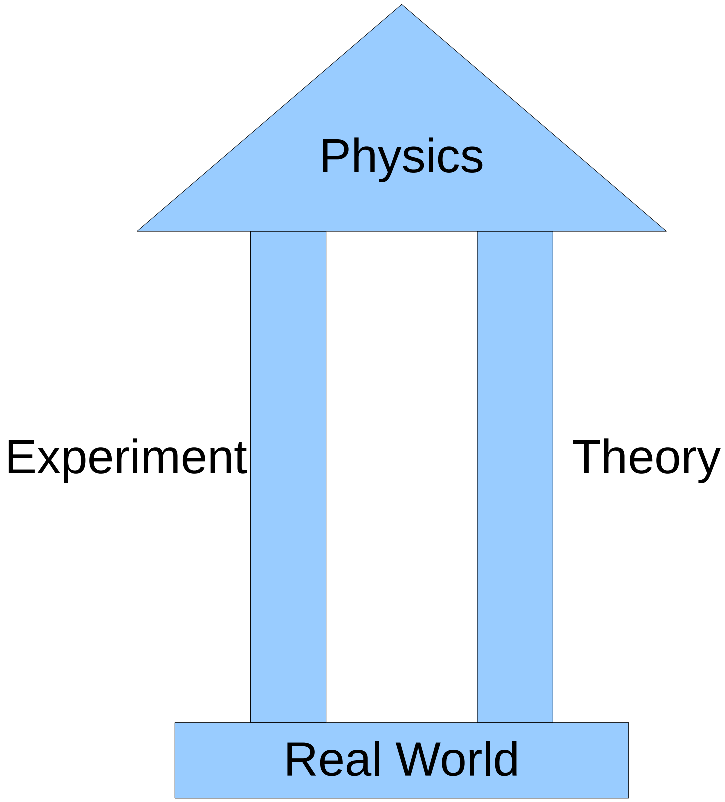
Scientific Machine Learning
Simulation Basics

Kristian Boroz

Contents

- Basics
- FDTD-Method
  - General Approach
  - Advanced Topics
  - Technical Aspects
- Applications
- Summary

Basics



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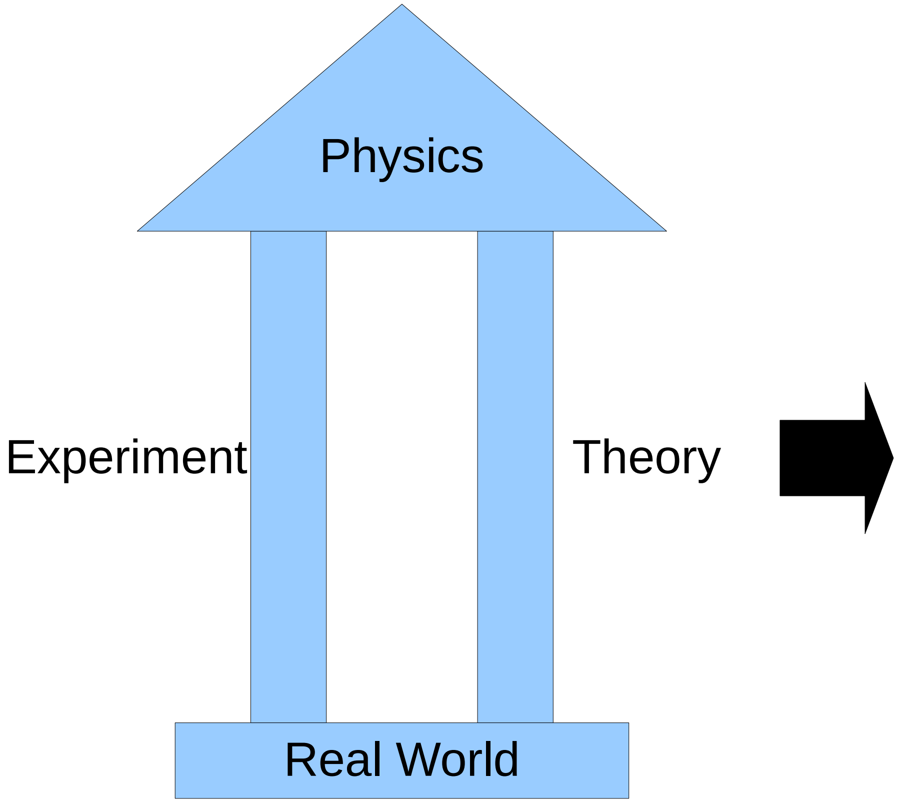

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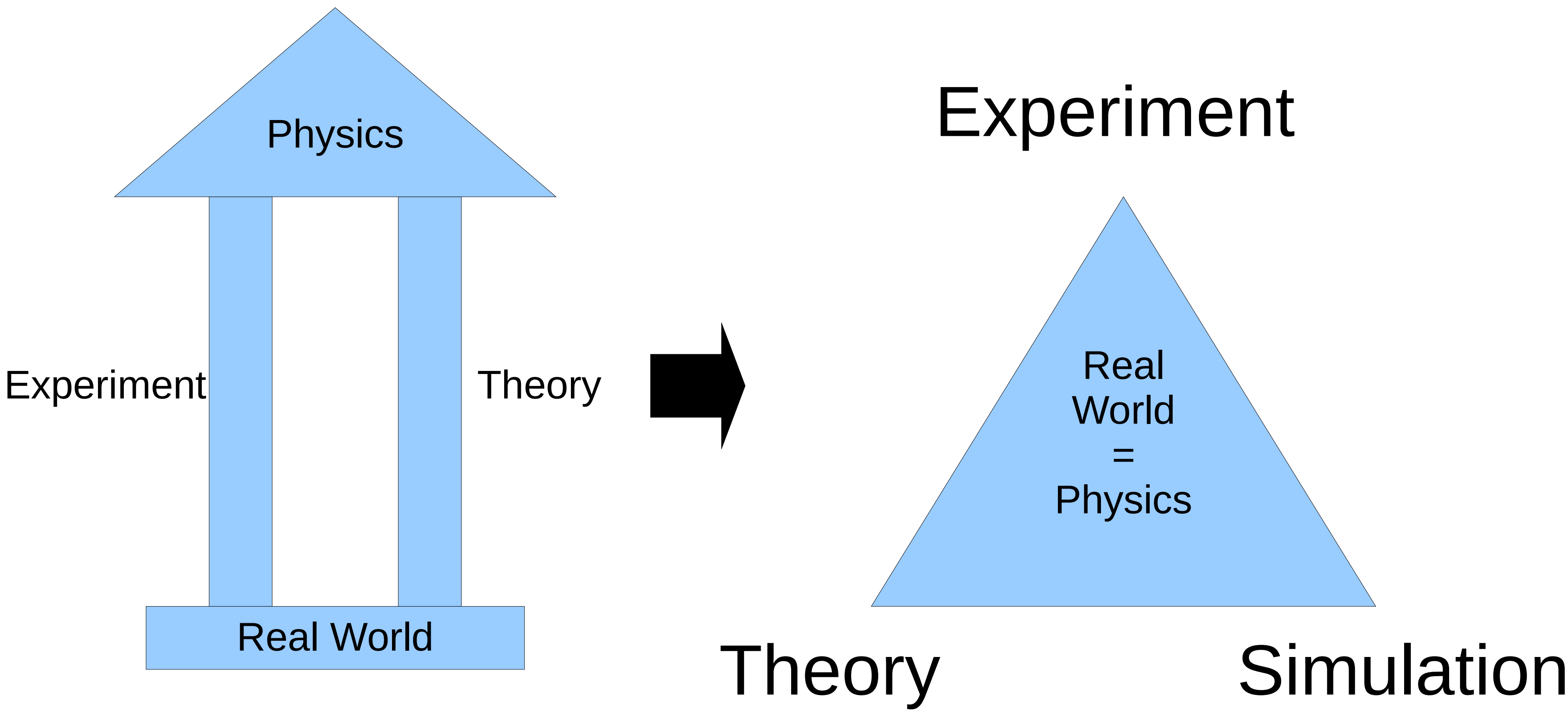
Physics
Experiment
Theory
Real World
Experiment
Real
World
=
Physics
Theory
Simulation

Basics

Basics

How to solve these problems?

Basics

- Analytical Solutions:

- Numerical Solutions:

Basics

- Analytical Solutions:
  - Fourier, Laplace methods…..
  - Green´s Functions
  - …
- Numerical Solutions:

Basics

- Analytical Solutions:
  - Fourier, Laplace methods…..
  - Green´s Functions
  - …
- Numerical Solutions:
  - Integral Approaches:
  - Differential Approaches:

Basics

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  - Fourier, Laplace methods…..
  - Green´s Functions
  - …
- Numerical Solutions:
  - Integral Approaches:
    - MoM,...
  - Differential Approaches:
    - FD, FEM, FVM,...

FDTD-METHOD

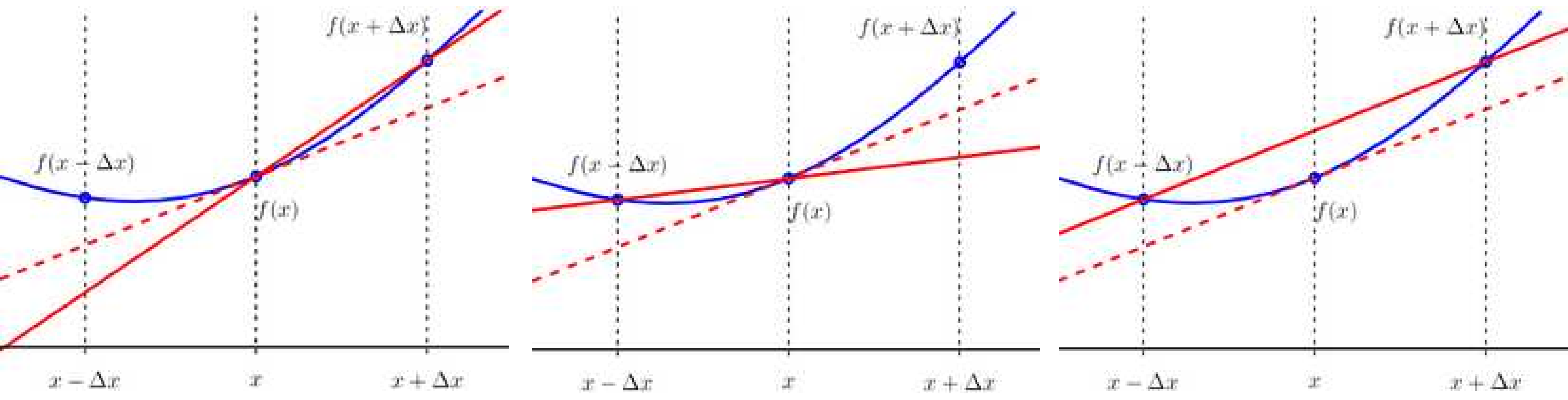
FDTD-METHOD

- Finite-Difference-Time-Domain = FDTD
- Approximation - Discretisation

$$f'(x) = \lim_{dx \to 0} \frac{f(x + dx)}{dx} + O(dx)$$

FDTD-METHOD

- Finite-Difference-Time-Domain = FDTD
- Approximation - Discretisation



$$\left.\frac{df(x)}{dx}\right|_x = \frac{f(x+dx)-f(x)}{dx}$$

$$error \sim O(dx)$$

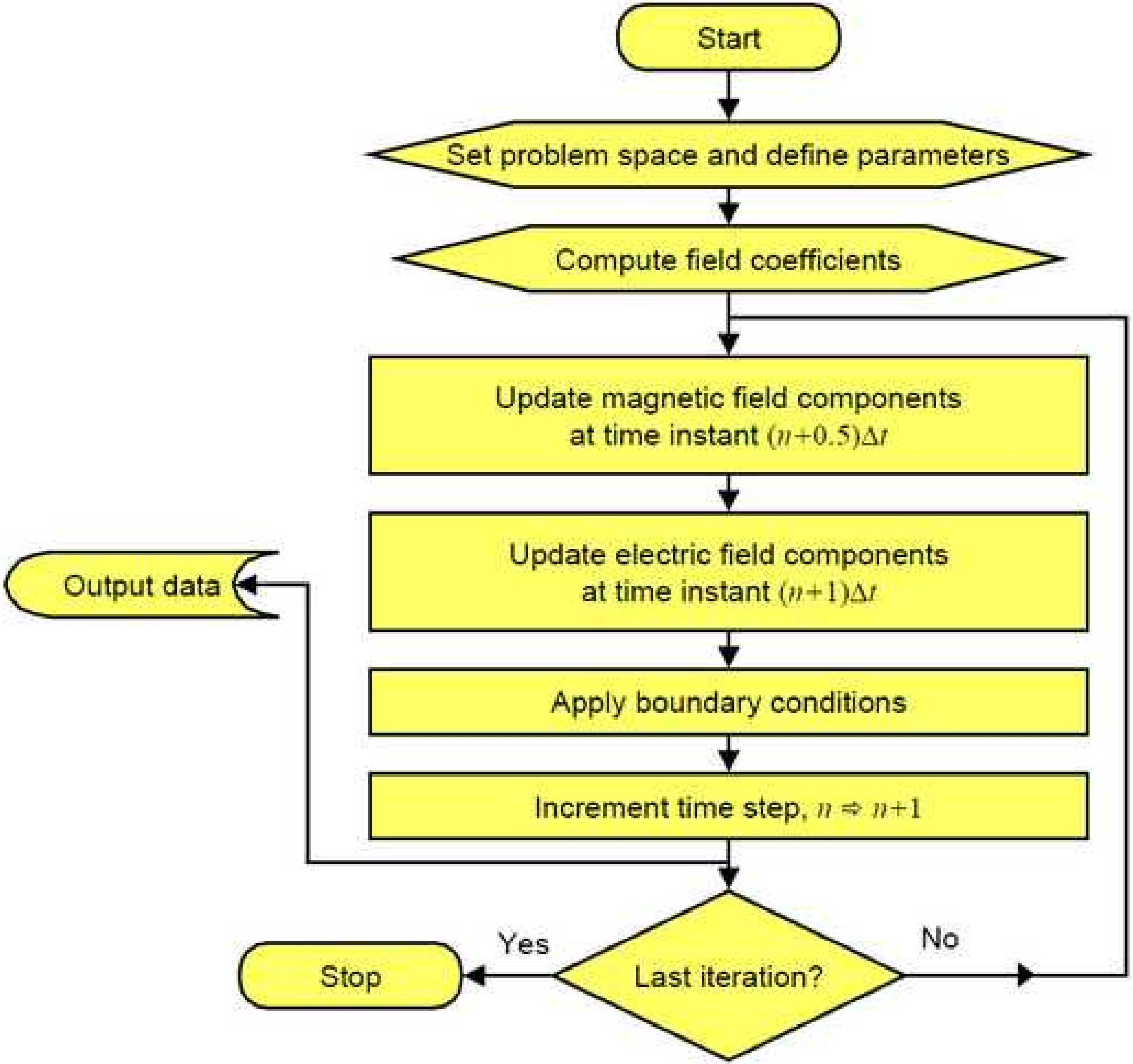
$$\left.\frac{df(x)}{dx}\right|_x = \frac{f(x)-f(x-dx)}{dx}$$

$$error \sim O(dx)$$

$$\left.\frac{df(x)}{dx}\right|_x = \frac{f(x+\frac{dx}{2})-f(x-\frac{dx}{2})}{dx}$$

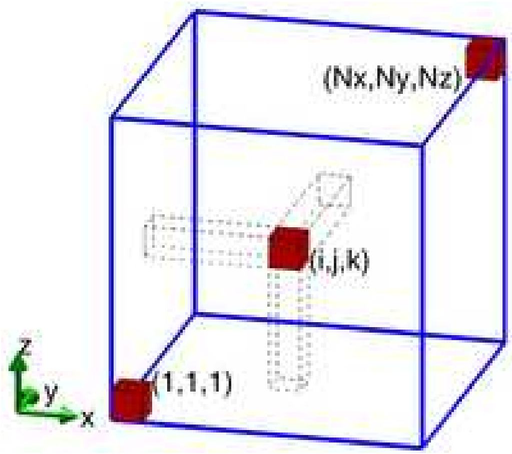
$$error \sim O((dx)^2)$$

FDTD-METHOD



Start
Set problem space and define parameters
Compute field coefficients
Update magnetic field components
at time instant $(n+0.5)\Delta t$
Update electric field components
at time instant $(n+1)\Delta t$
Output data
Apply boundary conditions
Increment time step, $n \Rightarrow n+1$
Yes
No
Stop
Last iteration?

FDTD-METHOD



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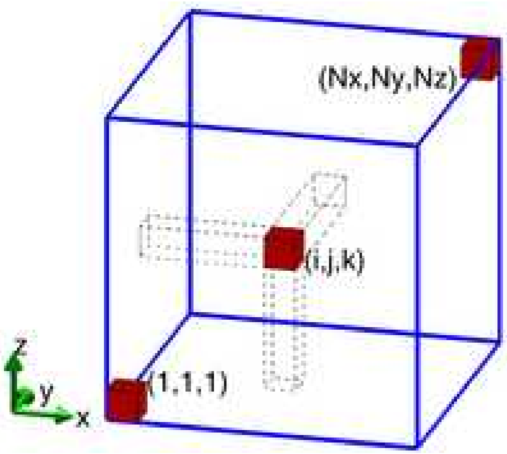

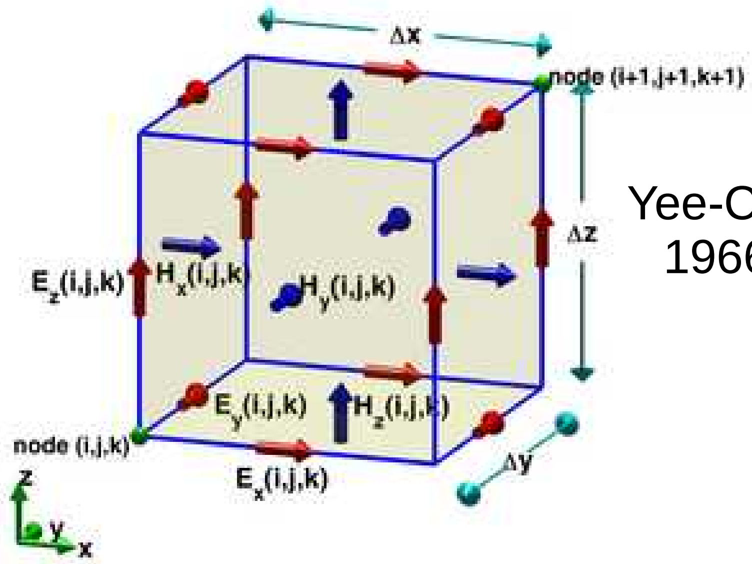

Yee-Cell
1966

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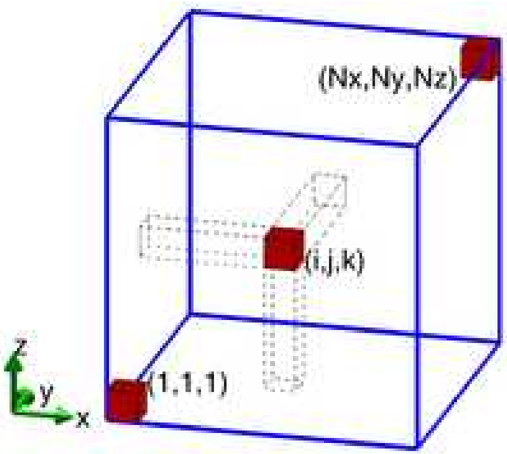
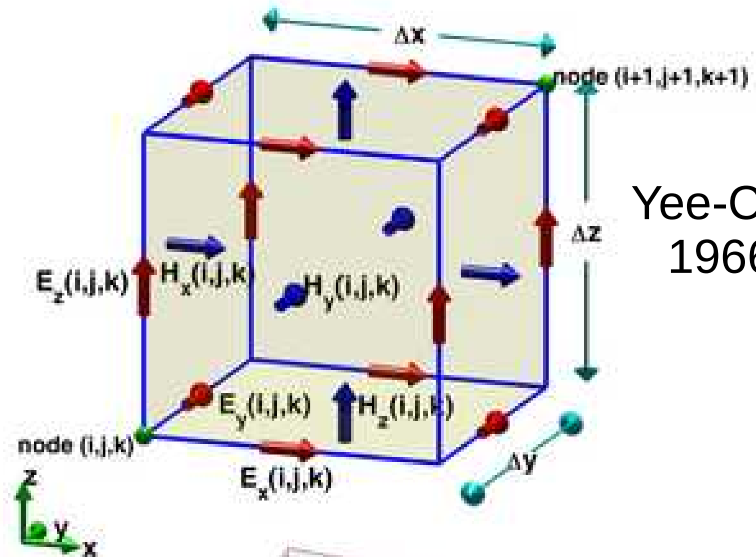
FDTD-METHOD





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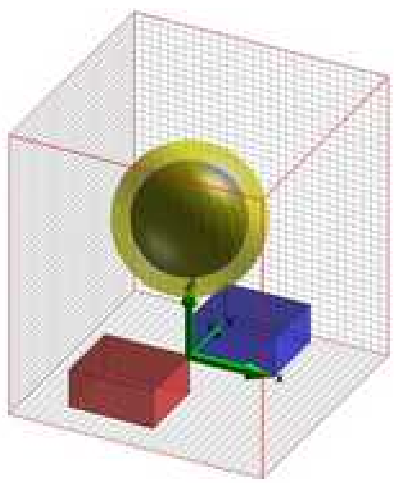

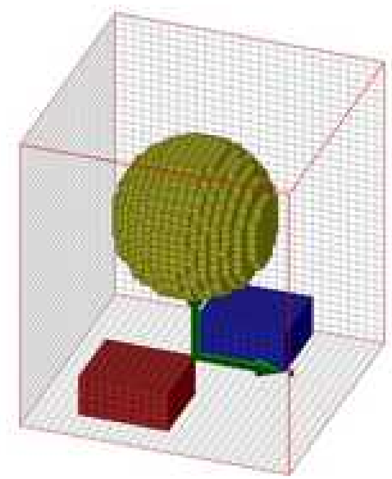

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FDTD-METHOD

- Starting from Maxwell´s Equations:

$$\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t} - \sigma_M \vec{H} \qquad \nabla \times \vec{H} = -\varepsilon \frac{\partial \vec{E}}{\partial t} - \sigma \vec{E}$$

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$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu_x}\left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \sigma_{Mx} H_x\right) \qquad \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_z}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma_z E_z\right)$$

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$$E_x^n\left(i+\frac{1}{2}, j, k\right) = E_x\left(\left(i+\frac{1}{2}\right)\Delta x, j\Delta y, k\Delta z, n\Delta t\right)$$

$$E_y^n\left(i, j+\frac{1}{2}, k\right) = E_y\left(i\Delta x, \left(j+\frac{1}{2}\right)\Delta y, k\Delta z, n\Delta t\right)$$

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FDTD-METHOD

$$H_x^{n+\frac{1}{2}}\left(i,j+\frac{1}{2},k+\frac{1}{2}\right)=\frac{\mu_x-0,5\Delta t\sigma_{Mx}}{\mu_x+0,5\Delta t\sigma_{Mx}}H_x^{n-\frac{1}{2}}\left(i,j+\frac{1}{2},k+\frac{1}{2}\right)$$

$$+\frac{\Delta t}{\mu_x+0,5\Delta t\sigma_{Mx}}\left(\frac{E_y^n\left(i,j+\frac{1}{2},k+\frac{1}{2}\right)-E_y^n\left(i,j+\frac{1}{2},k\right)}{\Delta z}-\frac{E_z^n\left(i,j+\frac{1}{2},k+\frac{1}{2}\right)-E_z^n\left(i,j,k+\frac{1}{2}\right)}{\Delta y}\right)$$

$$E_x^{n+1}\left(i+\frac{1}{2},j,k\right)=\frac{\varepsilon_x-0,5\Delta t\sigma_x}{\varepsilon_x+0,5\Delta t\sigma_x}E_x^n\left(i+\frac{1}{2},j,k\right)$$

$$+\frac{\Delta t}{\varepsilon_x+0,5\Delta t\sigma_x}\left(\frac{H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2},j+\frac{1}{2},k\right)-H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2},j-\frac{1}{2},k\right)}{\Delta y}-\frac{H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right)-H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right)}{\Delta z}\right)$$

FDTD-METHOD

- Advanced Topics
  - Numerical Stability
  - Boundary Conditions
    - ABC, PML, PEC, PMC,...
  - Improvements of FDTD
    - Nonuniform Mesh
    - Farfield-Calculations

FDTD-METHOD

- Advanced Topics
  - Numerical Stability

$$c\Delta t \leq \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

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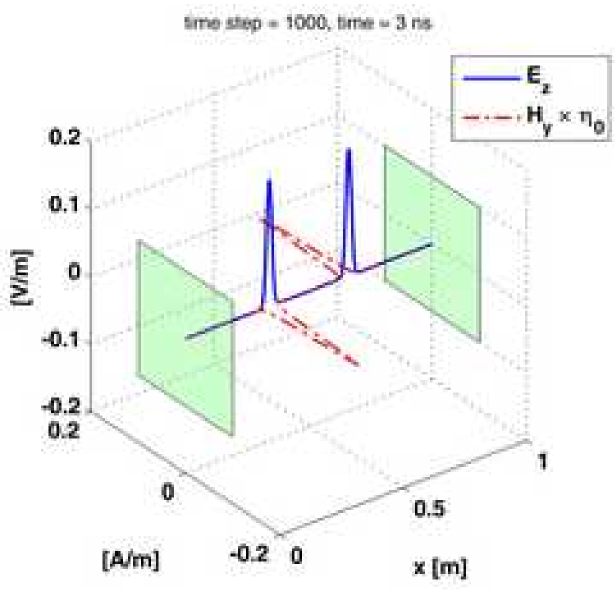

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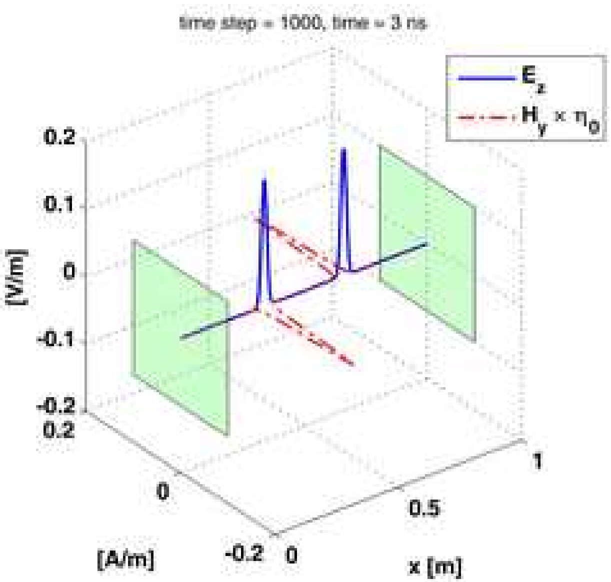

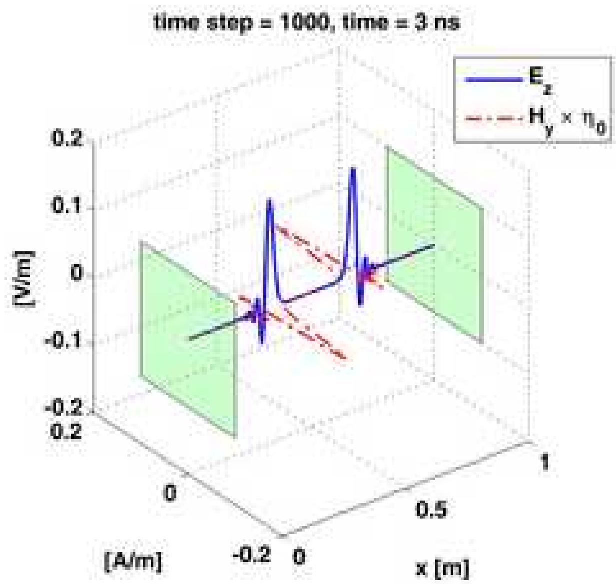

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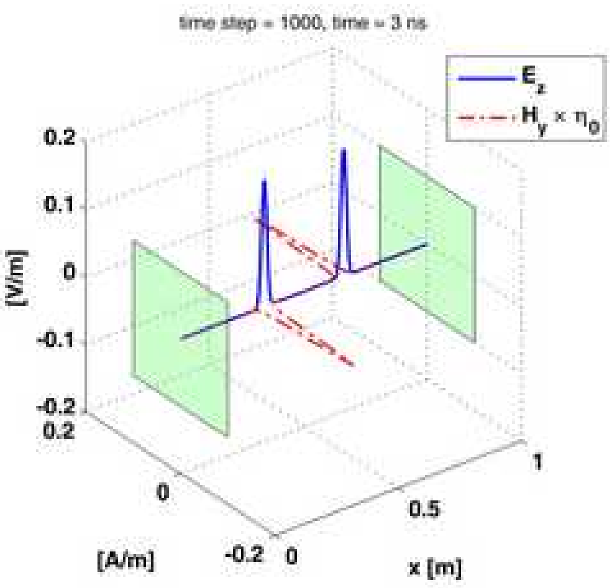

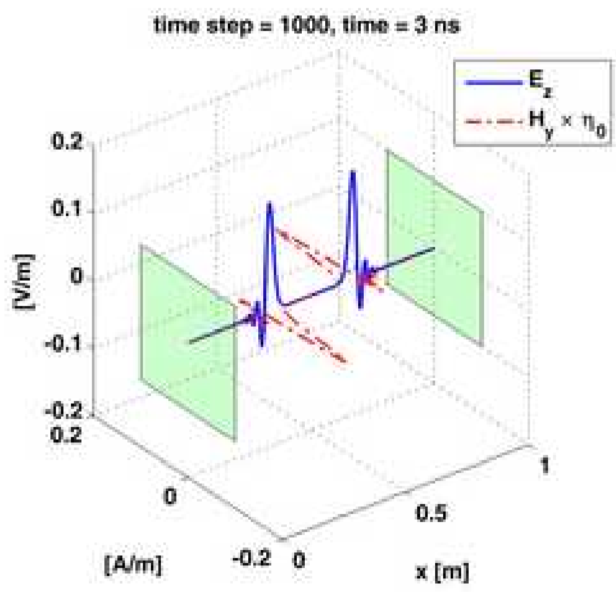

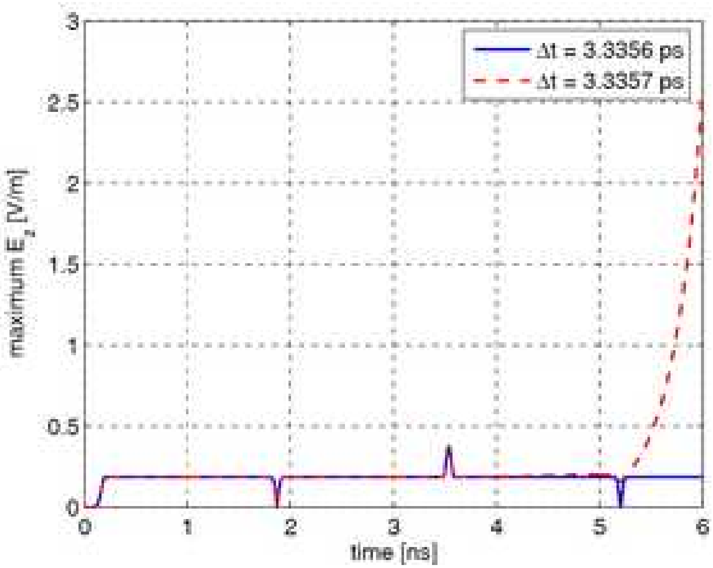

FDTD-METHOD

- Advanced Topics
  - Numerical Stability
  - Boundary Conditions

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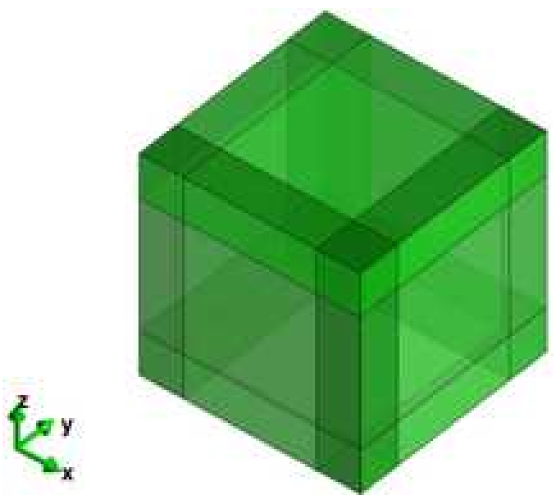

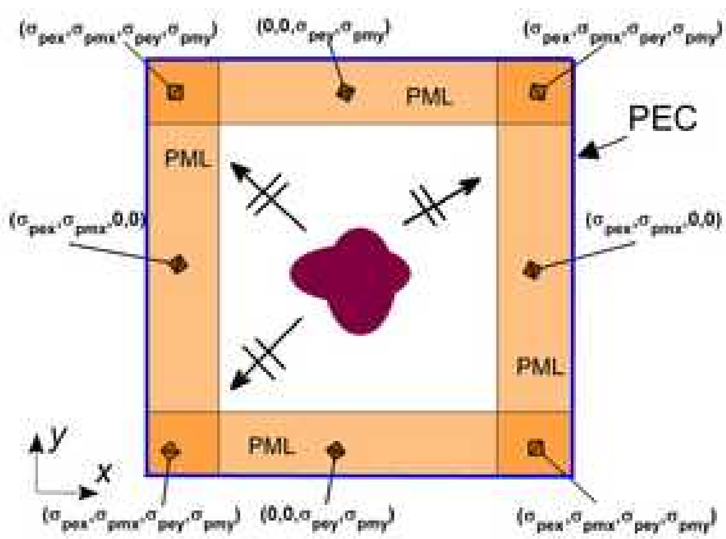

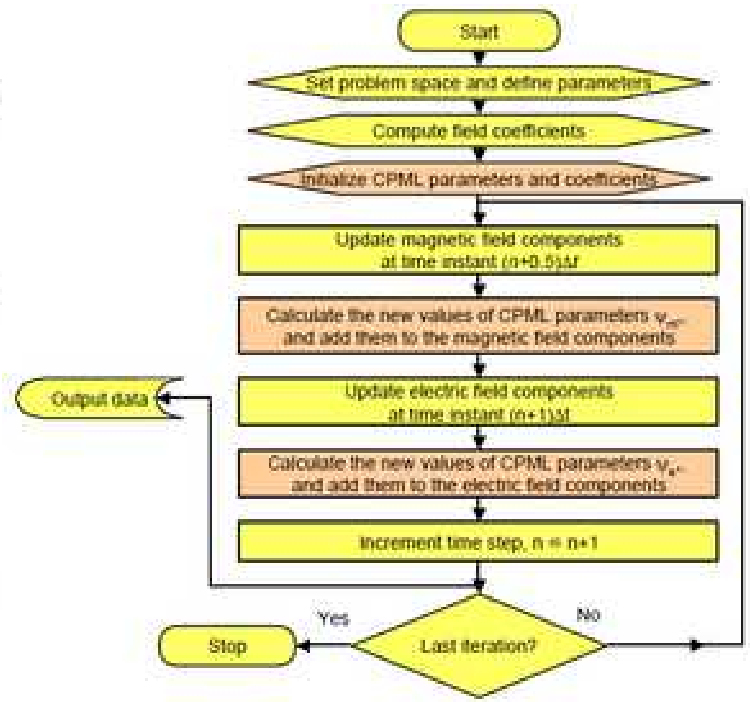

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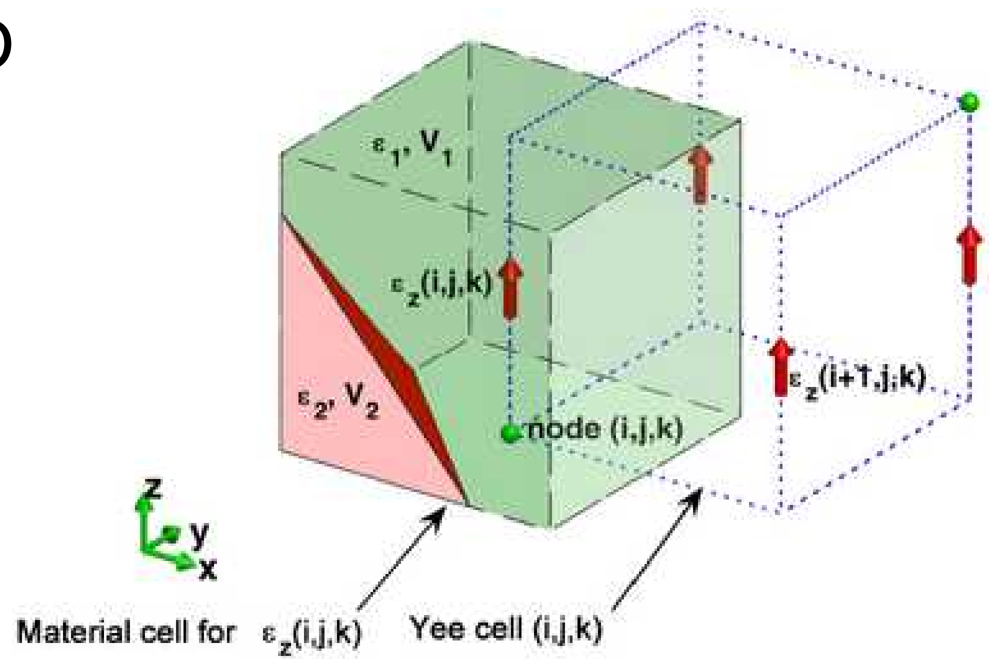

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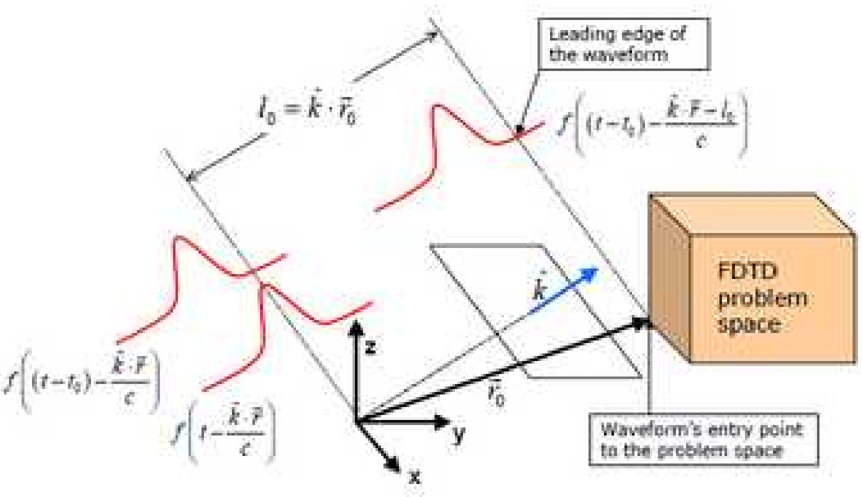

FDTD-METHOD

- Technical Aspects

FDTD-METHOD

- Technical Aspects
  - Problem of Discretisation
  - Parallelisation
  - Computersystems

FDTD-METHOD

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  - Problem of Discretisation
    - Stability-Criterion
      - Small Grid-Size = a lot of Memory = CPU-Time

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FDTD-METHOD

- Technical Aspects
  - Parallelisation
    - Loops and Vectorisation

FDTD-METHOD

- Technical Aspects
  - Computersystems
    - 4-Core-CPU
    - 24GB-RAM

      ~2000€

    - 4x12-Core-CPU
    - Up to 512 GB-RAM

      ~30000€

FDTD-METHOD

- Technical Aspects
  - Computersystems
    - GPU-Computing

FDTD-METHOD

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    - Graphic-Cards ~500-1000€

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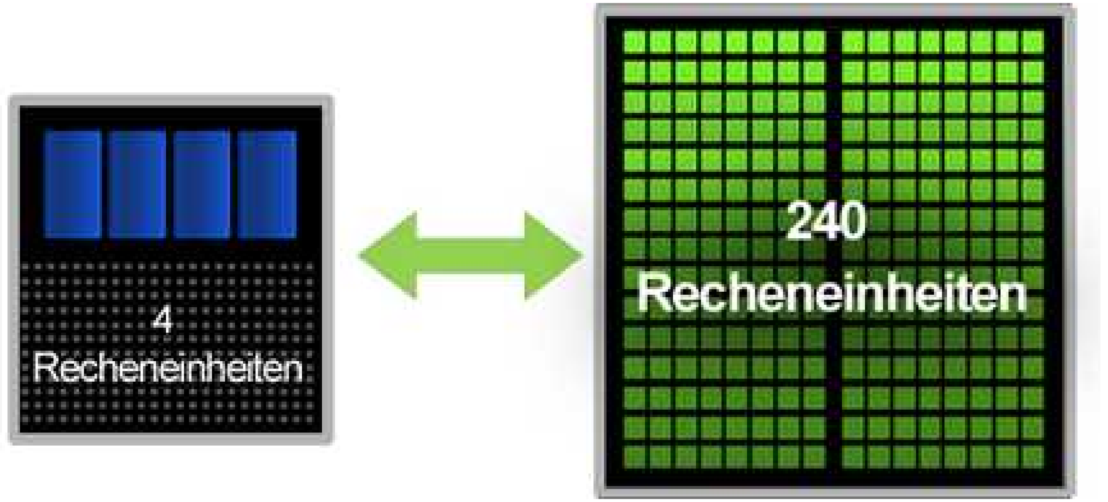

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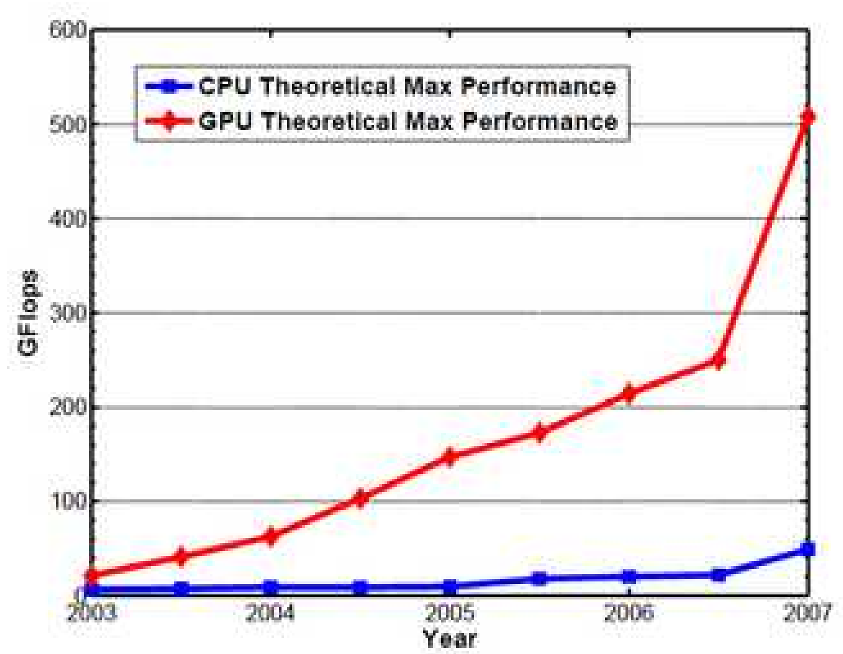

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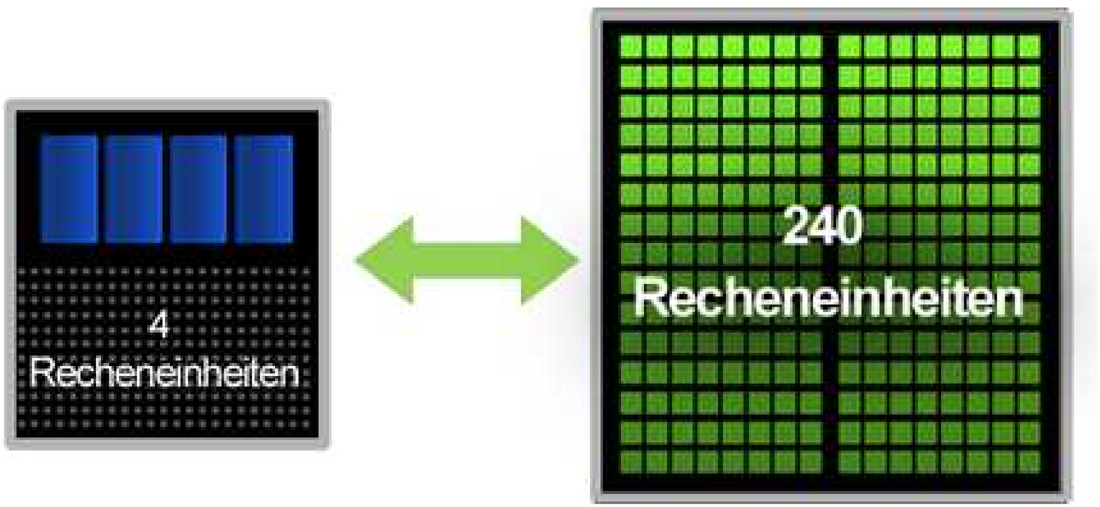

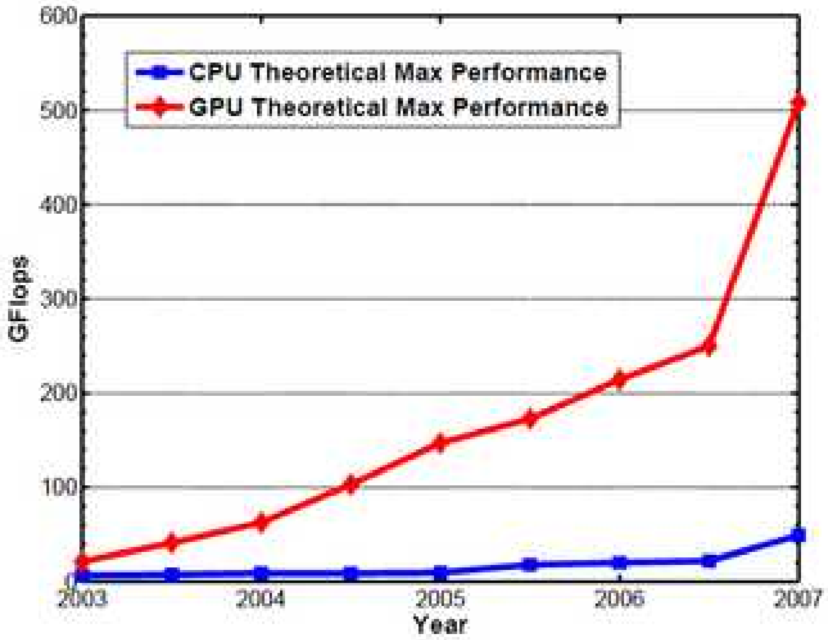

FDTD-METHOD

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    - Software-Solutions

FDTD-METHOD

- Technical Aspects
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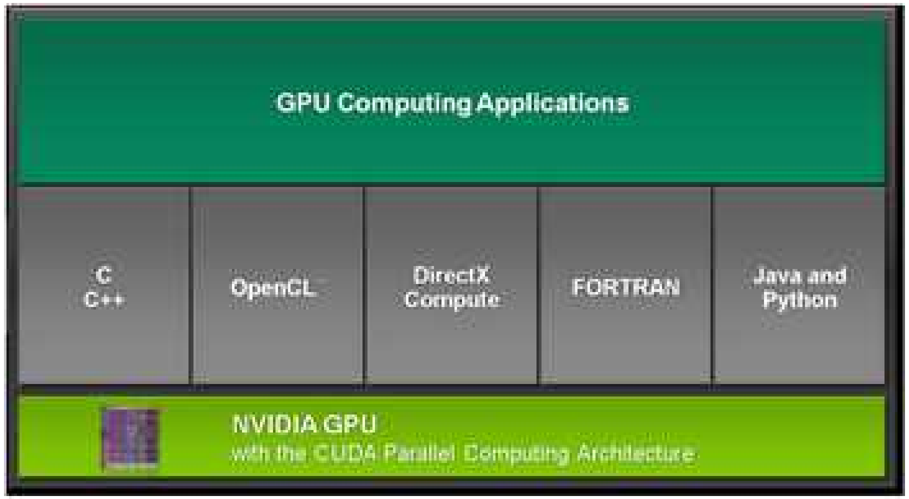
    - GPU-Computing
    - Software-Solutions
      - Nvidia-CUDA-Programming
      - AMD/ATI-Stream
      - OpenCL
      - EM-Photonics
      - GPUmat
      - Accelereyes-GPU-Matlab-Computing - Jacket



AI REVOLUTION !?!?

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- generative AI
- image processing / computer vision
- speech recognition
- translation
- scientific knowledge discovery
- forecasting and prediction
- etc.

<u>AI REVOLUTION !?!?</u>

AI REVOLUTION !?!?

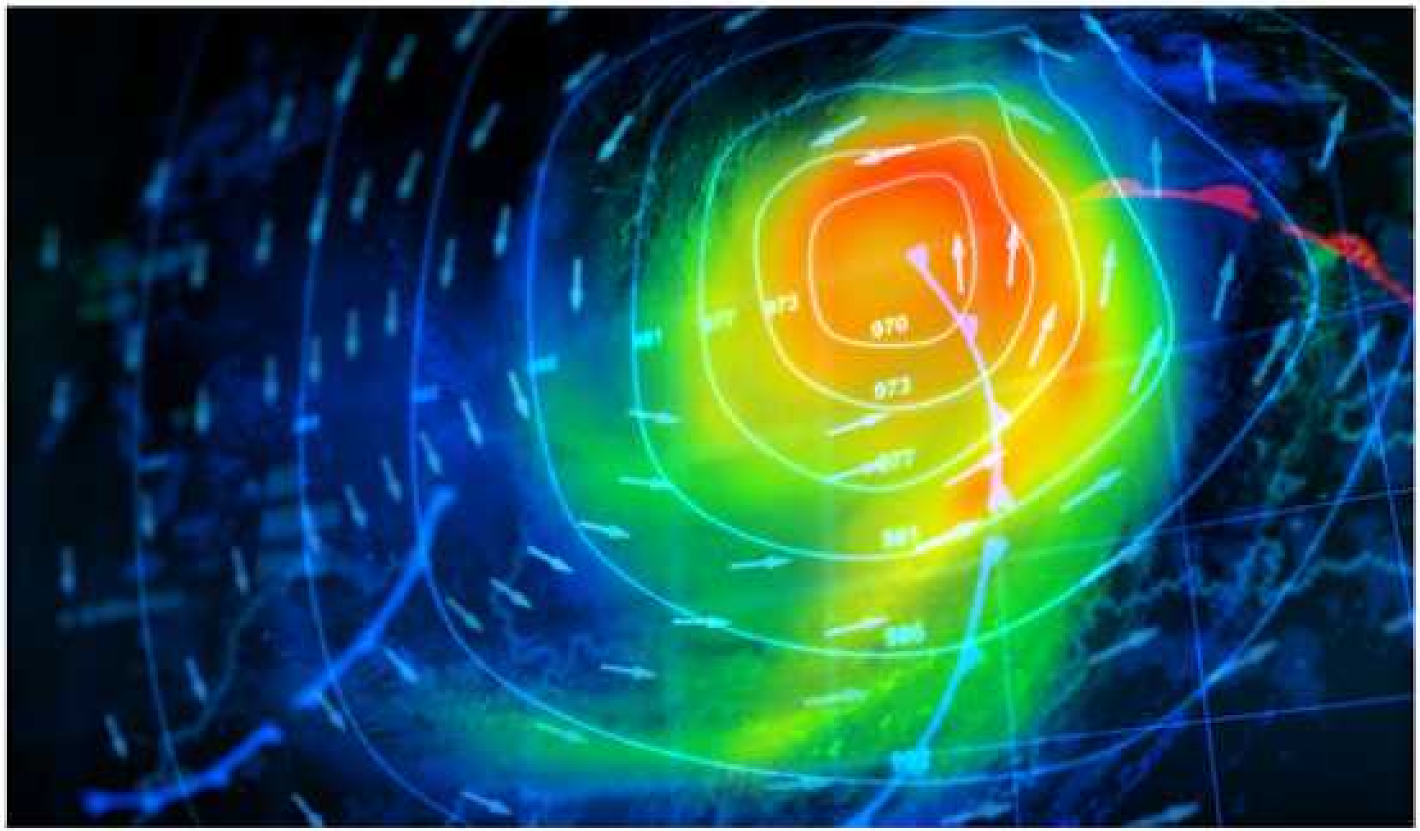
- Developed by Google DeepMind
- Predicts 3D protein structures from string of amino acids

Outcomes

- Accelerating drug discovery and design
- Accelerating research on cancer / Alzheimer's / etc.
- Supporting enzyme engineering for sustainability

Authors awarded 2024 Nobel Prize in Chemistry

AI REVOLUTION !?!?



AI REVOLUTION !?!?

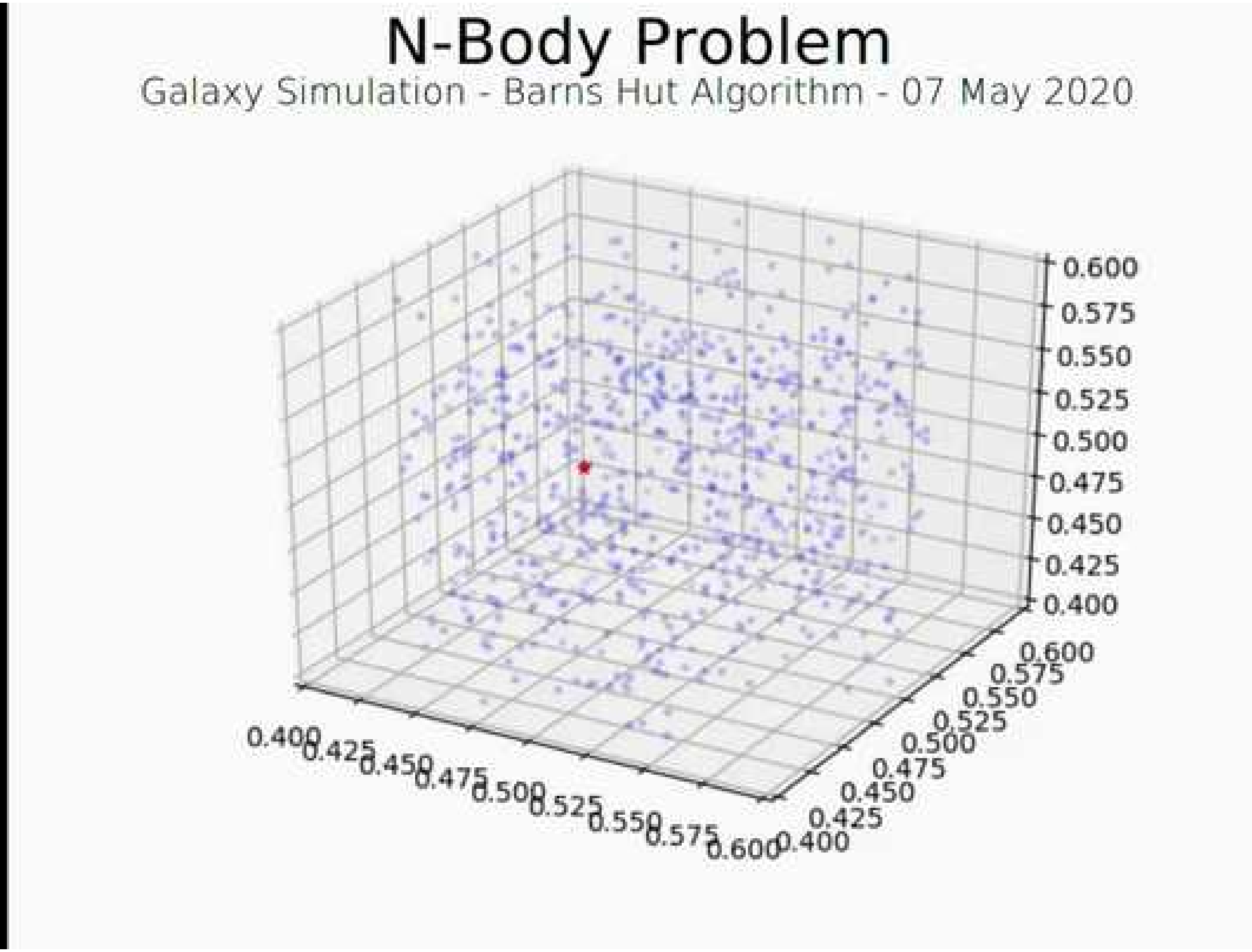
"ECMWF's weather forecasting model is considered the gold standard for medium-term weather forecasting...Google DeepMind claims to beat it 90% of the time..."

"Traditional forecasting models are big, complex computer algorithms based on atmospheric physics and take hours to run. AI models can create forecasts in just seconds."

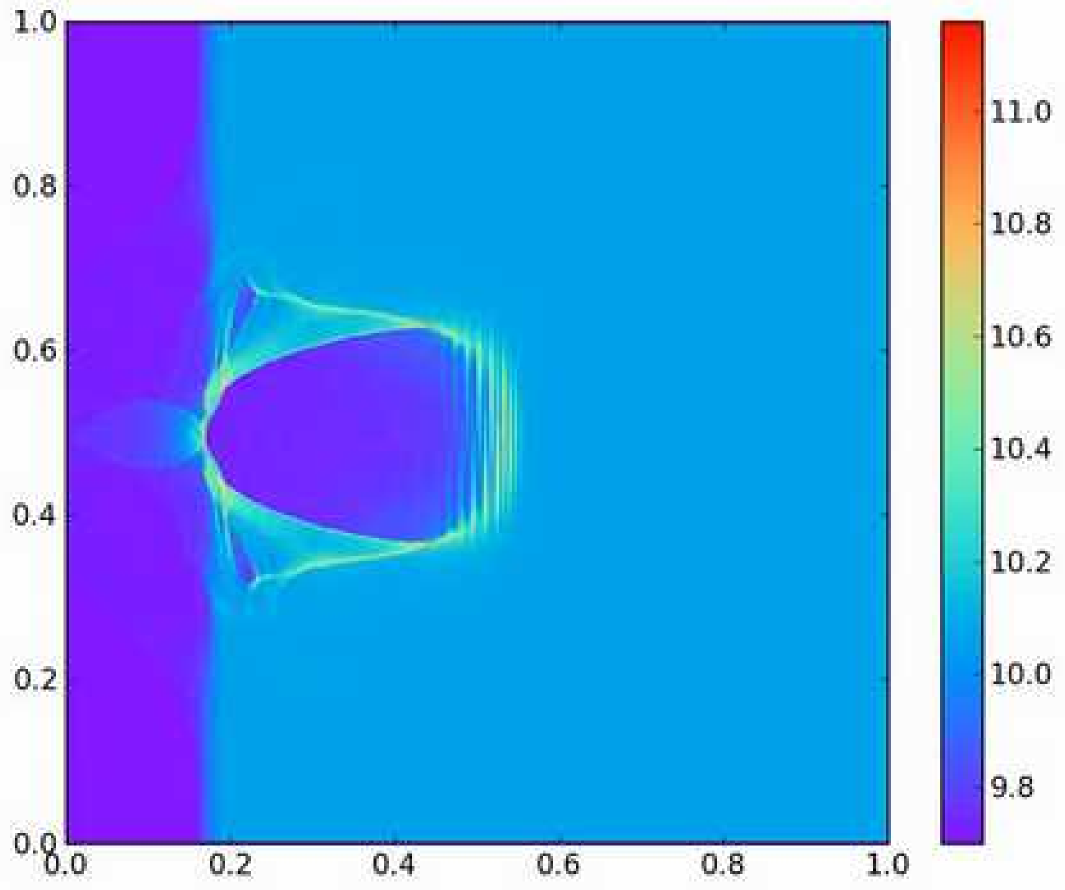
Source: MIT Technology Review July 2024

Applications & Results

Applications & Results



Applications & Results



Applications & Results

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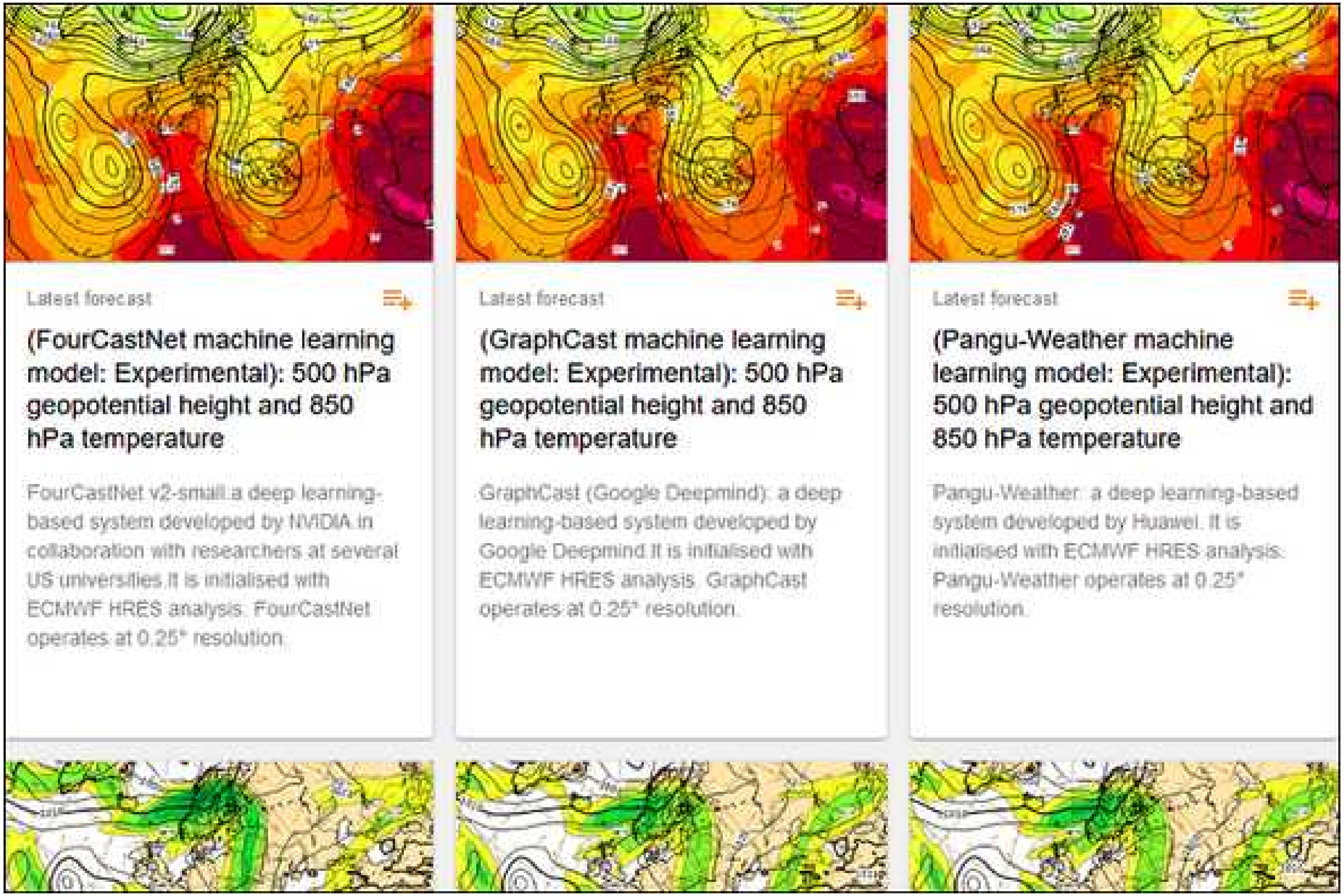
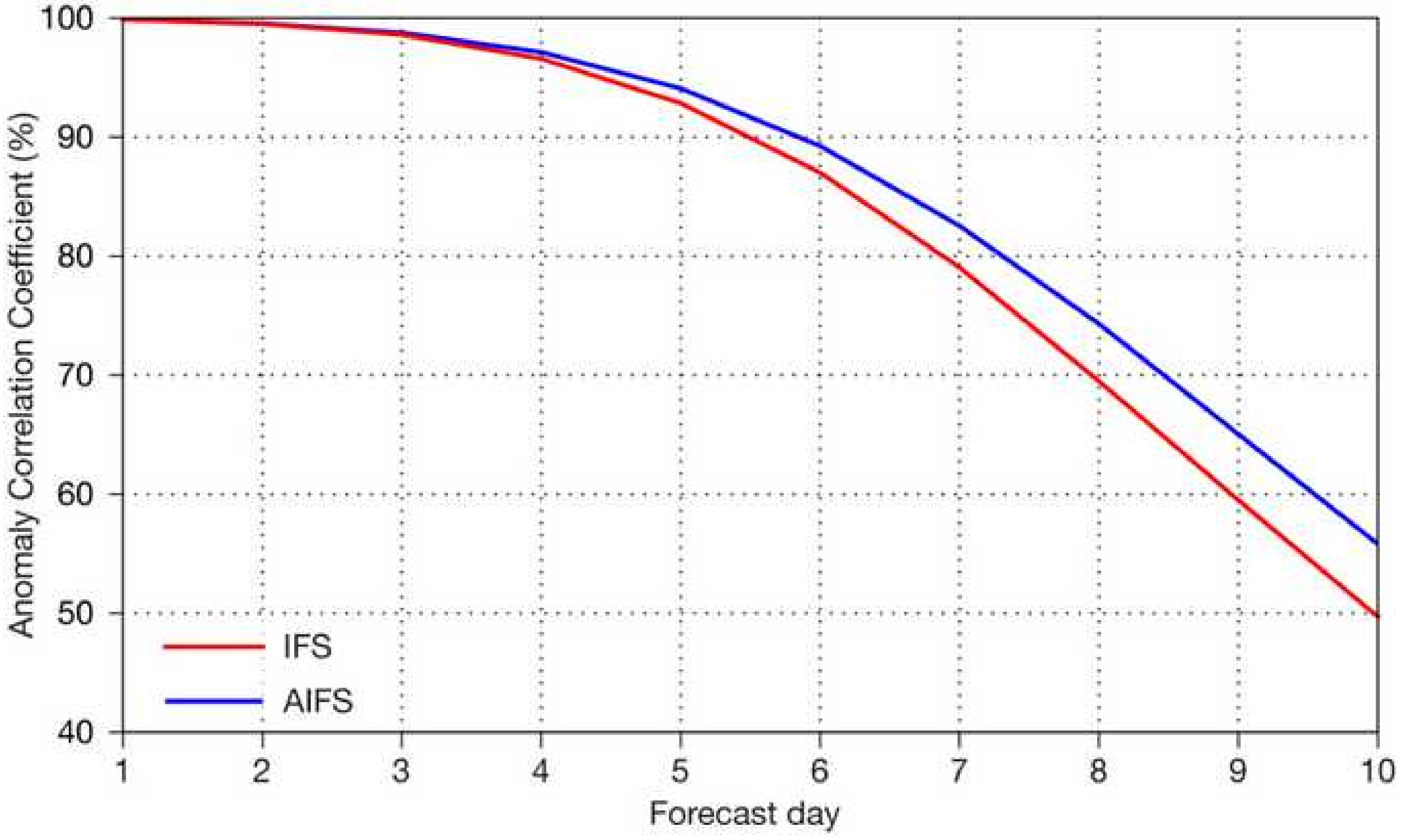
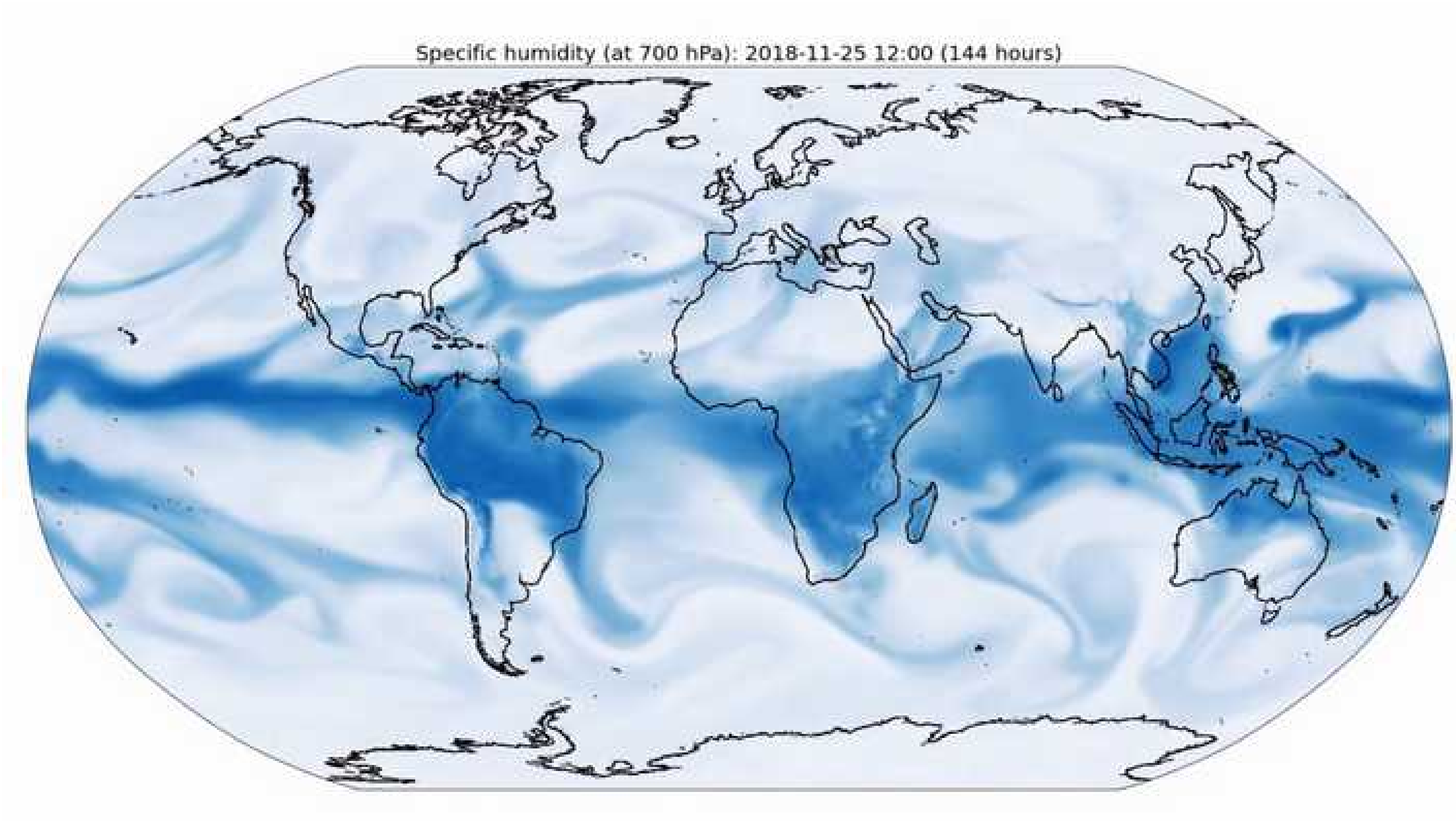


Applications & Results



Applications & Results



SCIENCE

Discovering new solutions to century-old problems in fluid dynamics

18 SEPTEMBER 2025

Yongji Wang, Sam Blackwell

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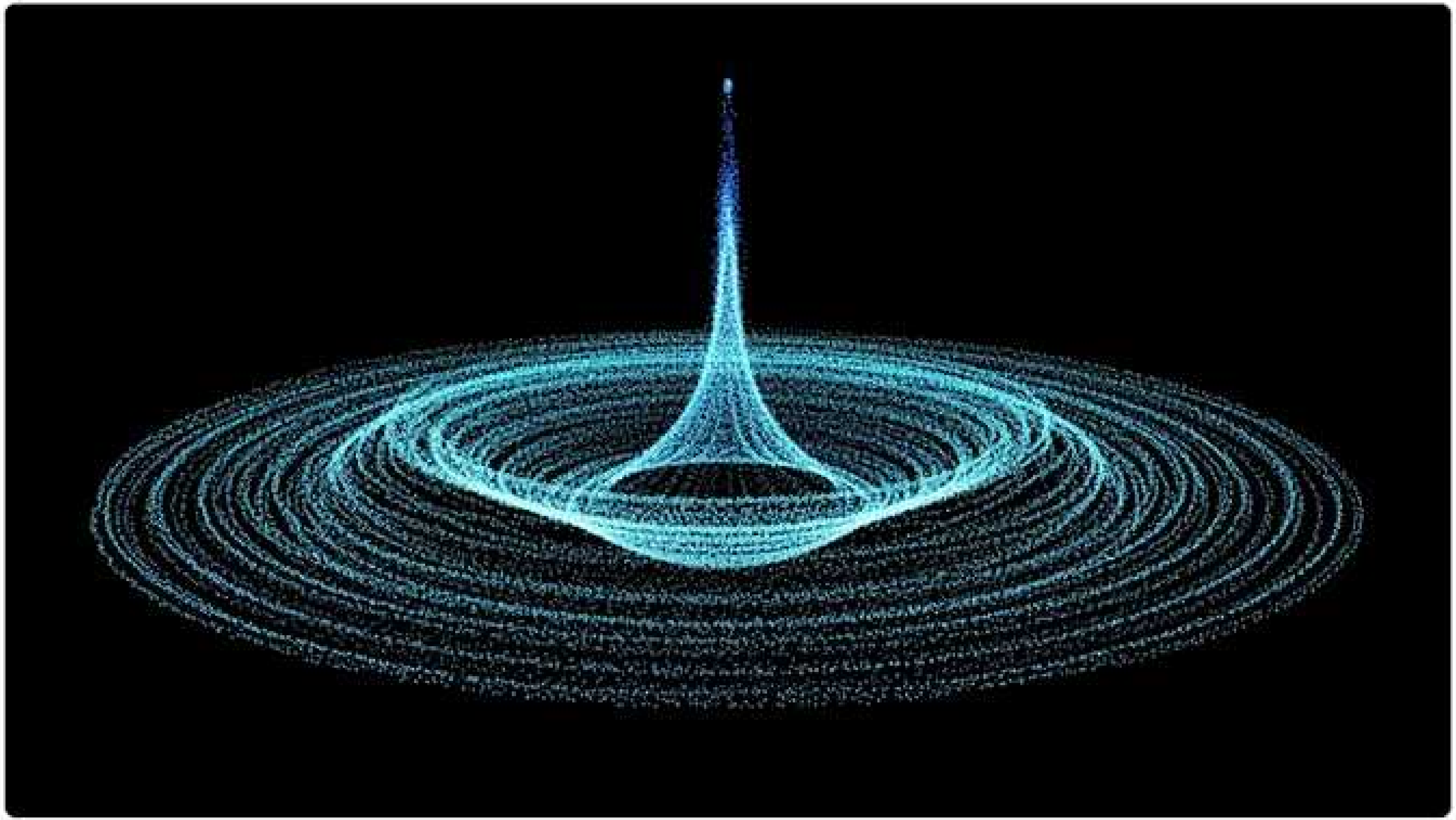

Summary

- FDTD-Simulations are a powerful Tool
  - Approximation by Discretisation
  - Boundary Conditions: PML, etc.
  - Technical Aspects: Gridsize, Memory, CPU-Time
- Comparison with experimental results

Material

- Taflove - Computational Electrodynamics: The Finite-Difference Time-Domain Method - Artech House Inc (2005)
- Wenhua - Parallel - Finite-Difference Time-Domain Method - Artech House Inc (2006)
- Sadiku - Numerical Techniques in Electromagnetics with MATLAB - Crc Pr Inc (2009)
- Elsherbeni - The Finite-Difference Time-Domain Method for Electromagnetics with MATLAB Simulations - Scitech Pub (2008)
- http://www.nvidia.com/object/cuda_home_new.html
- https://deepmind.google/discover/blog/discovering-new-solutions-to-century-old-problems-in-fluid-dynamics/
- https://github.com/google-deepmind/graphcast
- https://www.ecmwf.int/en/newsletter/178/news/aifs-new-ecmwf-forecasting-system

Questions & Comments

THANK YOU !!!