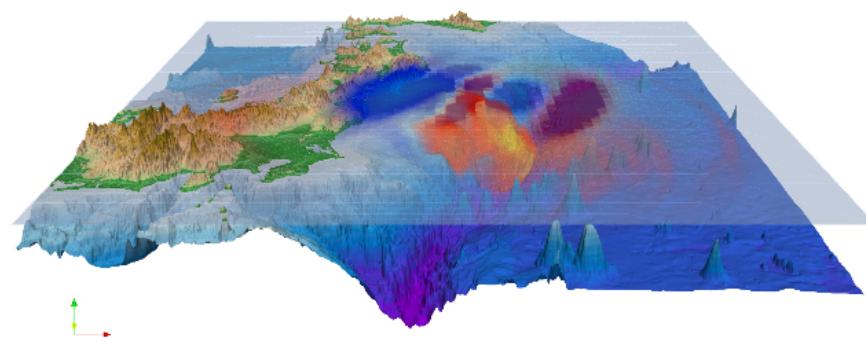


# Scientific Computing

Summer 2020

Jörn Behrens  
[joern.behrens@uni-hamburg.de](mailto:joern.behrens@uni-hamburg.de)



# Introduction

## Teacher



Prof. Dr. Jörn Behrens  
Urs Hamburg/CiSAP  
Grindelberg 5, Room 411 (4th floor)  
Bundesstraße 55, Room 12D (1st floor)  
Tel. (040) 42838 7734  
mail joern.behrens@uni-hamburg.de

[Show CV](#)  
[Research Interests](#)

## Outline

Scientific Computing Summer 2020

Date	
21.04.20	Introduction
22.04.20	Computer Architectures
02.05.20	Performance Assessment
12.05.20	Programming Models
13.05.20	Parallelization, Parallelization Strategies
20.05.20	SLAS
03.06.20	Break/Holidays
04.06.20	Computers, hardware and rendering
16.06.20	Iterative Methods
23.06.20	Various Methods
30.06.20	Introduction to domain decomposition
07.07.20	Additive and Multiplicative Schwarz Methods
14.07.20	Wrap-up

## Lecture Organization

Lectures:  
See videos on MIN Moodle, whenever you like  
Tuesdays, 14:15-15:00, weekly Zoom Chat

Exercises:  
5 Exercise Sheets for working at home  
50% weight for final mark

Exams:  
Final Exam, 50% weight, either online or at UHH

## Aims

- Part 1:  
Computers, Hardware, Architectures, etc.
- Part 2:  
Examples of standard algorithms and optimization
- Part 3:  
Applications

# Teacher



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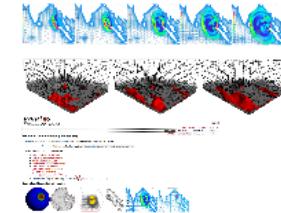
# *Teacher's Background*

## Short CV

since 2009 Prof. @ Uni Hamburg, KlimaCampus  
2006-2009 Head of Tsunami Group @ AWI, Adjunct Prof. @ Uni Bremen  
2003-2004 Visiting Scientist @ NCAR, Boulder, CO, USA  
1998-2006 Assistant Prof. and Lecturer @ TUM, Scientific Computing  
1996-1998 Post-Doc @ AWI  
1991-1996 PhD @ AWI: Adaptive Shallow Water SLM

## Research Interests

Adaptive Tsunami Modeling



Adaptive Atmospheric Modeling

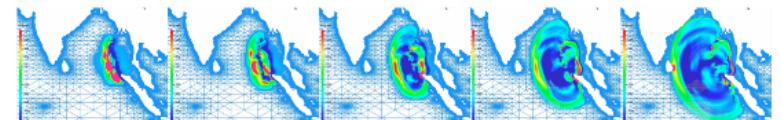
Grid Generation

# Short CV

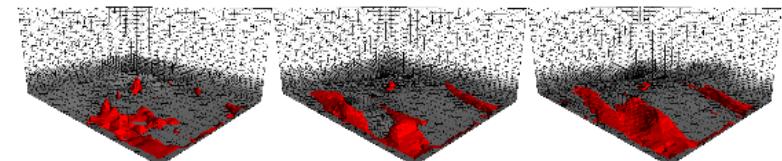
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# Research Interests

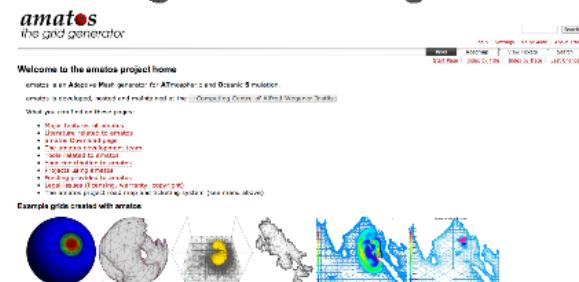
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Adaptive Atmospheric Modeling



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# *Aims*

## **Part1:**

Computers, Hardware, Architectures, etc.

## **Part 2:**

Examples of standard algorithms and optimization

## **Part 3:**

Applications

# *Outline*

## Scientific Computing Summer 2020

<b>Date</b>	<b>Lectures</b>
21.04.20	Introduction
28.04.20	Computer Architectures
05.05.20	Performance Assessment
12.05.20	Programming Models
19.05.20	Generic Parallelization Strategies
26.05.20	BLAS
02.06.20	Break/Holidays
09.06.20	Matrix structures and reordering
16.06.20	Iterative methods
23.06.20	Multigrid-Methods
30.06.20	Introduction to domain decomposition
07.07.20	Additive and Multiplicative Schwartz-Methods
14.07.20	Wrap-up

# Scientific Computing Terms and Definition

## Definition

Def: Scientific Computing  
"The field of study concerned with computing, mathematics and statistics, using quantitative analysis techniques and using computers to analyse and solve scientific problems" (University of Cambridge)

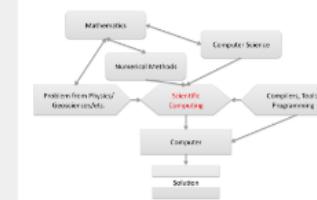
"The use of computing to solve scientific and engineering problems, often by the construction of models or simulations, or the construction of mathematical models of physical, chemical or biological processes" (Encyclopaedia)

- Computing
- Mathematical Model
- Scientific method

## 3 Columns of Knowledge



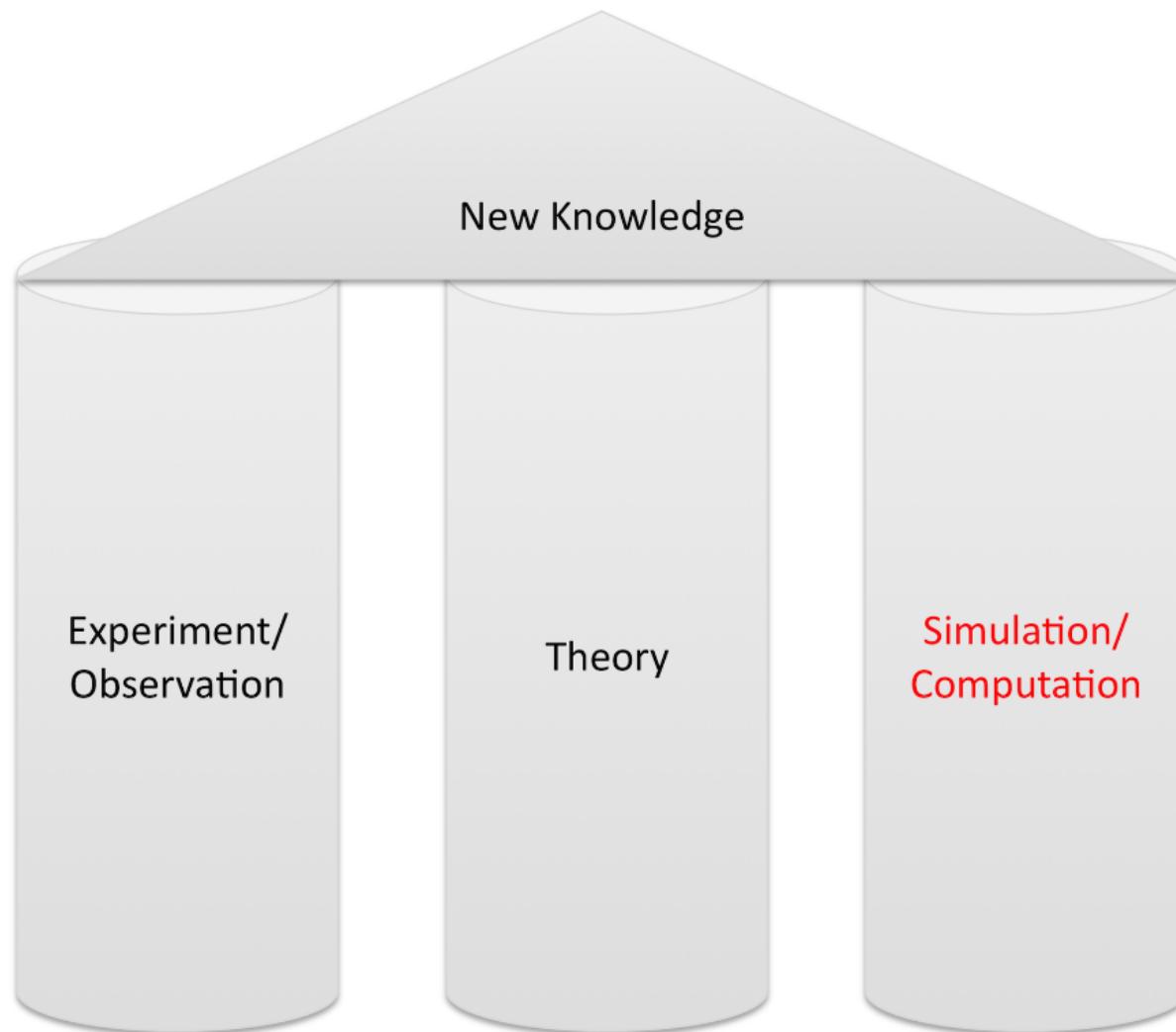
## Schematic



## Terms

- Mathematical Model Development
- Discretization
- Numerical Solution and Algorithm
- High Performance Computer
- Computing Architecture
- Performance Metrics
- Verification and Validation
- Visualization

# *3 Columns of Knowledge*

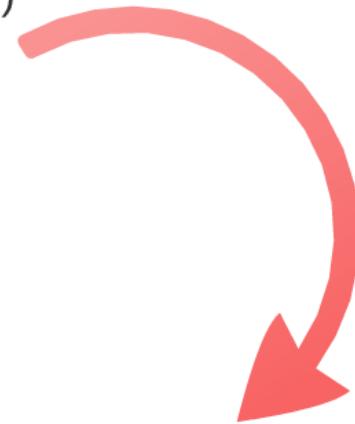


# *Definition*

## **Def: Scientific Computing**

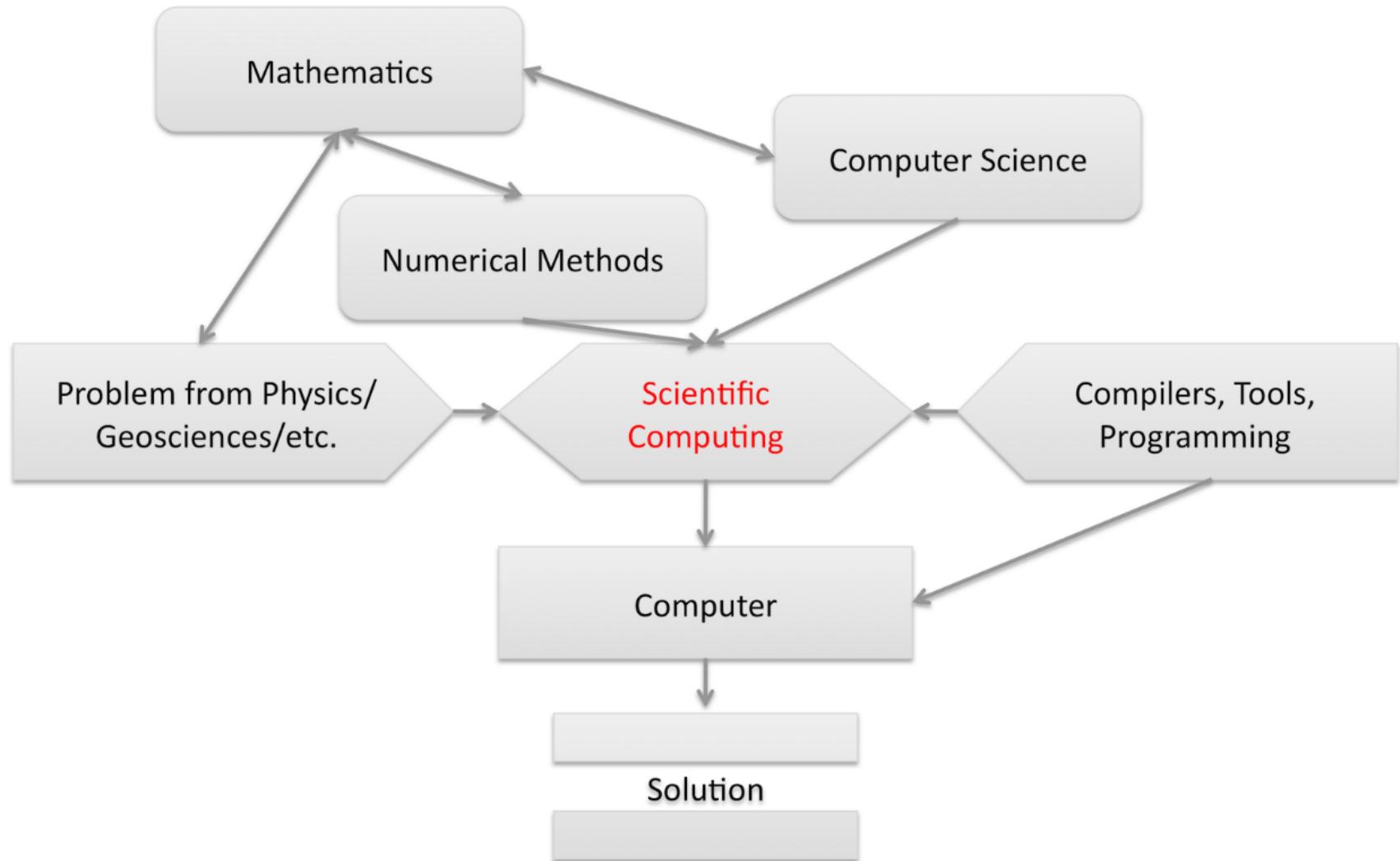
"The field of study concerned with constructing mathematical models and quantitative analysis techniques and using computers to analyze and solve scientific problems" (University of Cambridge)

"The use of computing to solve scientific and engineering problems, especially by means of simulation, or the construction of mathematical models of physical, chemical or biological processes" (Wictionary)



- Computing
- Mathematical Model
- Scientific method

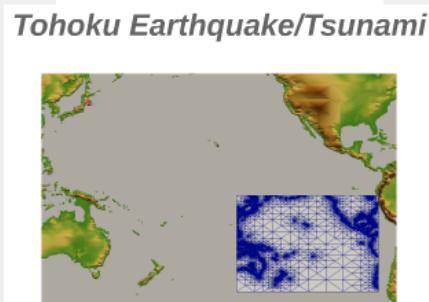
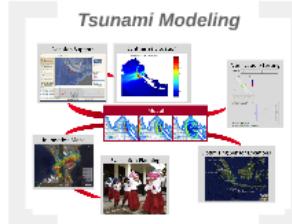
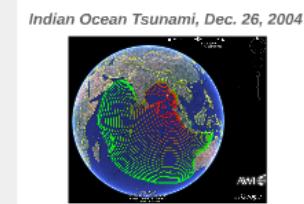
# Schematic



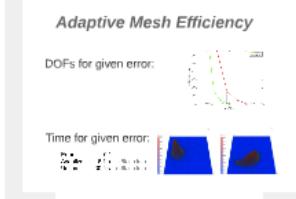
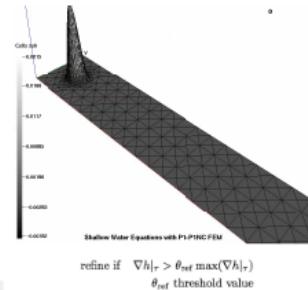
# *Terms*

- Mathematical Model Development
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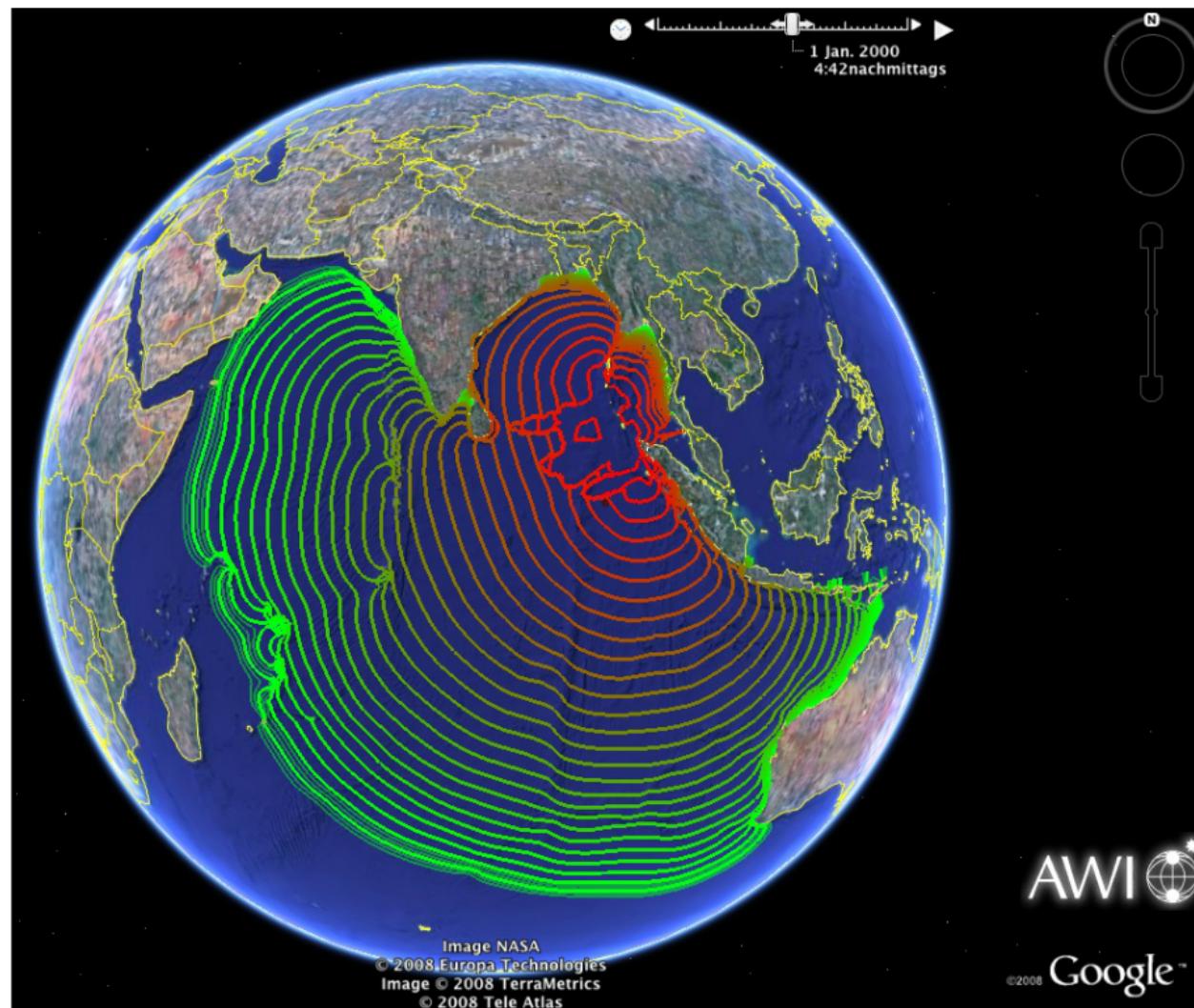
# Example: Tsunami Forecasting and Warning



## Adaptive Mesh Modeling



# *Indian Ocean Tsunami, Dec. 26, 2004*



# Inundation in Banda Aceh

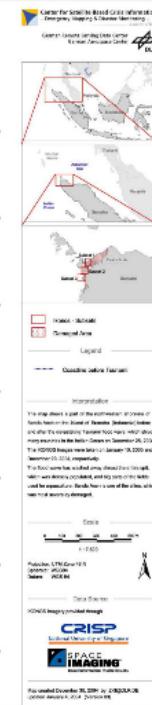


Indonesia - Banda Aceh Subset 1

IKONOS - January 10, 2003 - PRE-DISASTER IMAGE

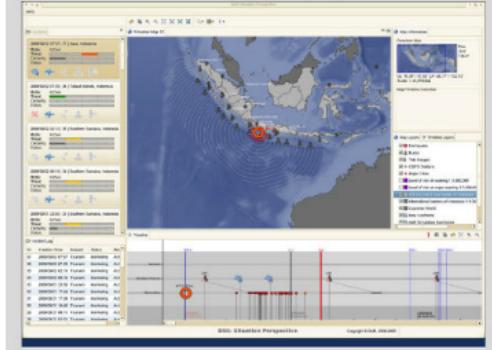


IKONOS - December 29, 2004 - POST-DISASTER IMAGE

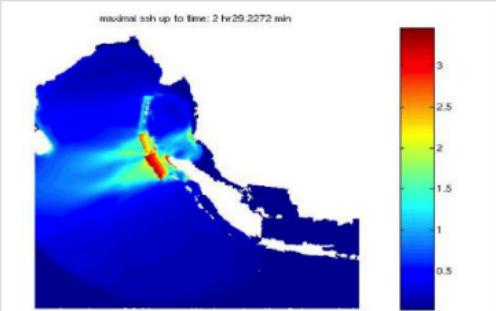


# Tsunami Modeling

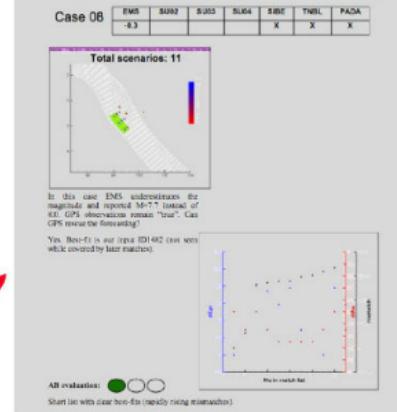
Decision Support



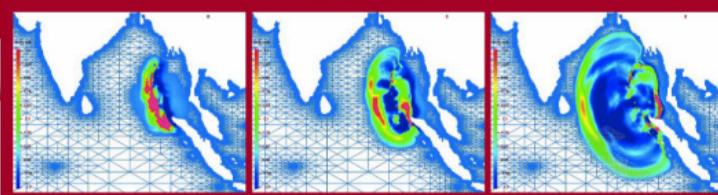
Synthesize Situation



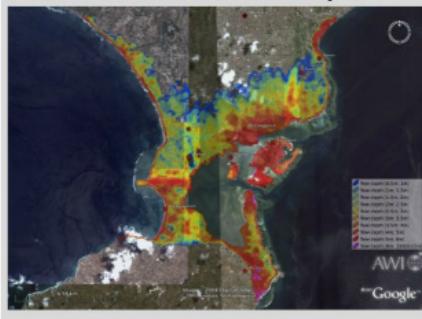
Verification/Testing



Model



Inundation Maps



Evacuation Planning



Optimizing Sensor Locations



# Modeling

## Equations

Non-linear shallow water equations:

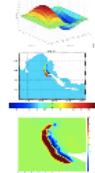
$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + g \nabla \eta = R,$$
$$\frac{\partial \eta}{\partial t} + \nabla \cdot (H \mathbf{v}) = 0.$$

$$R = -f \mathbf{k} \times \mathbf{v} - r H^{-1} |\mathbf{v}| \mathbf{v} + H^{-1} \nabla (K_h H \nabla \mathbf{v})$$

- Terms:  
• Coriolis  
• Bottom friction  
• Viscosity (Smagorinsky approach)

## Initial Conditions

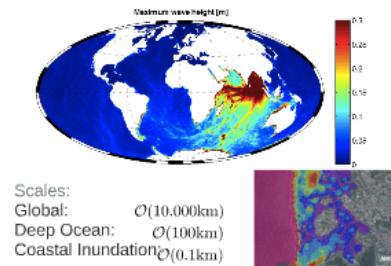
- Simplified
- Okada Plate Model
- Complex



## Boundary Conditions

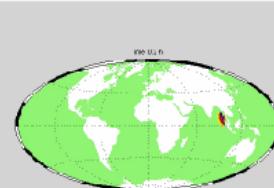


## Multi-Scale Characteristic



Scales:  
Global:  $\mathcal{O}(10.000\text{km})$   
Deep Ocean:  $\mathcal{O}(100\text{km})$   
Coastal Inundation:  $\mathcal{O}(0.1\text{km})$

## Extent



# *Equations*

Non-linear shallow water equations:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + g \nabla \eta = R,$$

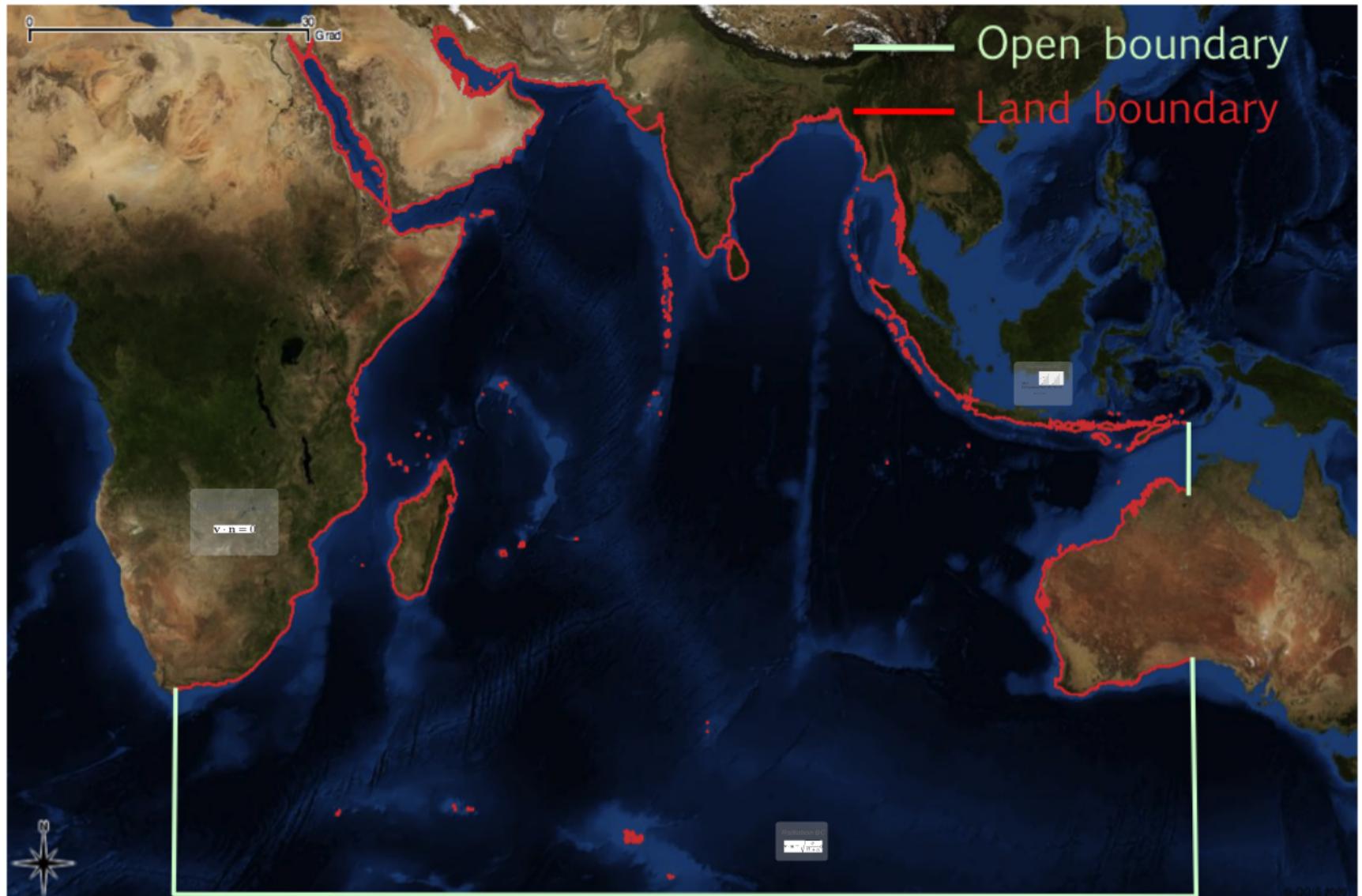
$$\frac{\partial \eta}{\partial t} + \nabla \cdot (H \mathbf{v}) = 0.$$

$$R = -f \mathbf{k} \times \mathbf{v} - r H^{-1} \mathbf{v} |\mathbf{v}| + H^{-1} \nabla (K_h H \nabla \mathbf{v})$$

Terms:

- Coriolis
- Bottom friction
- Viscosity (Smagorinsky approach)

# Boundary Conditions



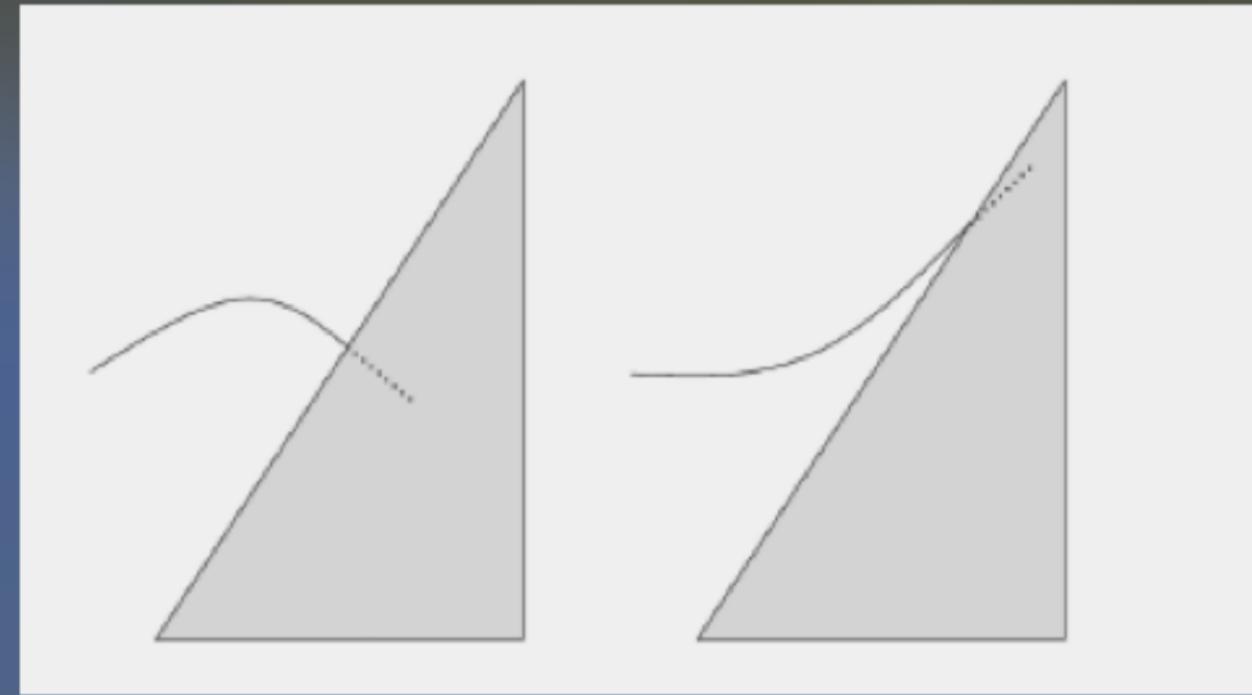
# *Reflecting BC*

$$\mathbf{v} \cdot \mathbf{n} = 0$$

# *Inundation BC*

Idea:

Extrapolate from dry to wet



On triangular grids:

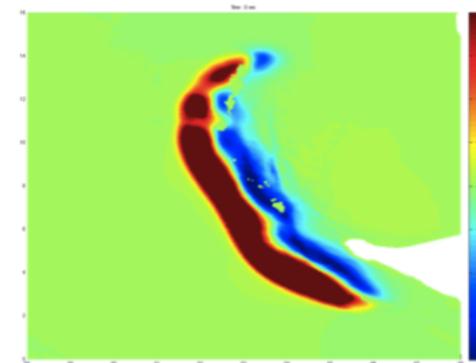
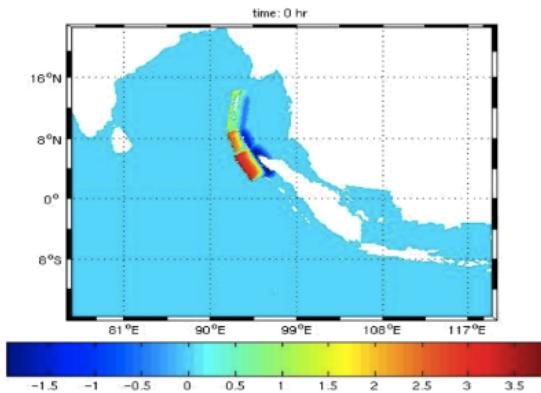
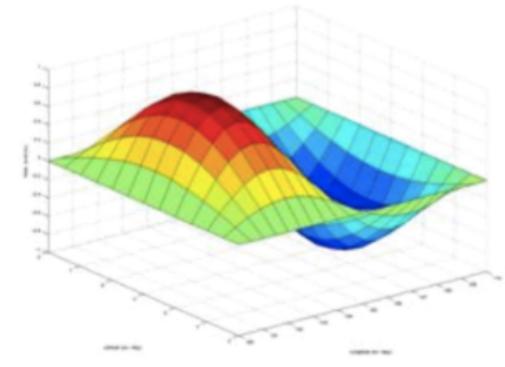


# *Radiation BC*

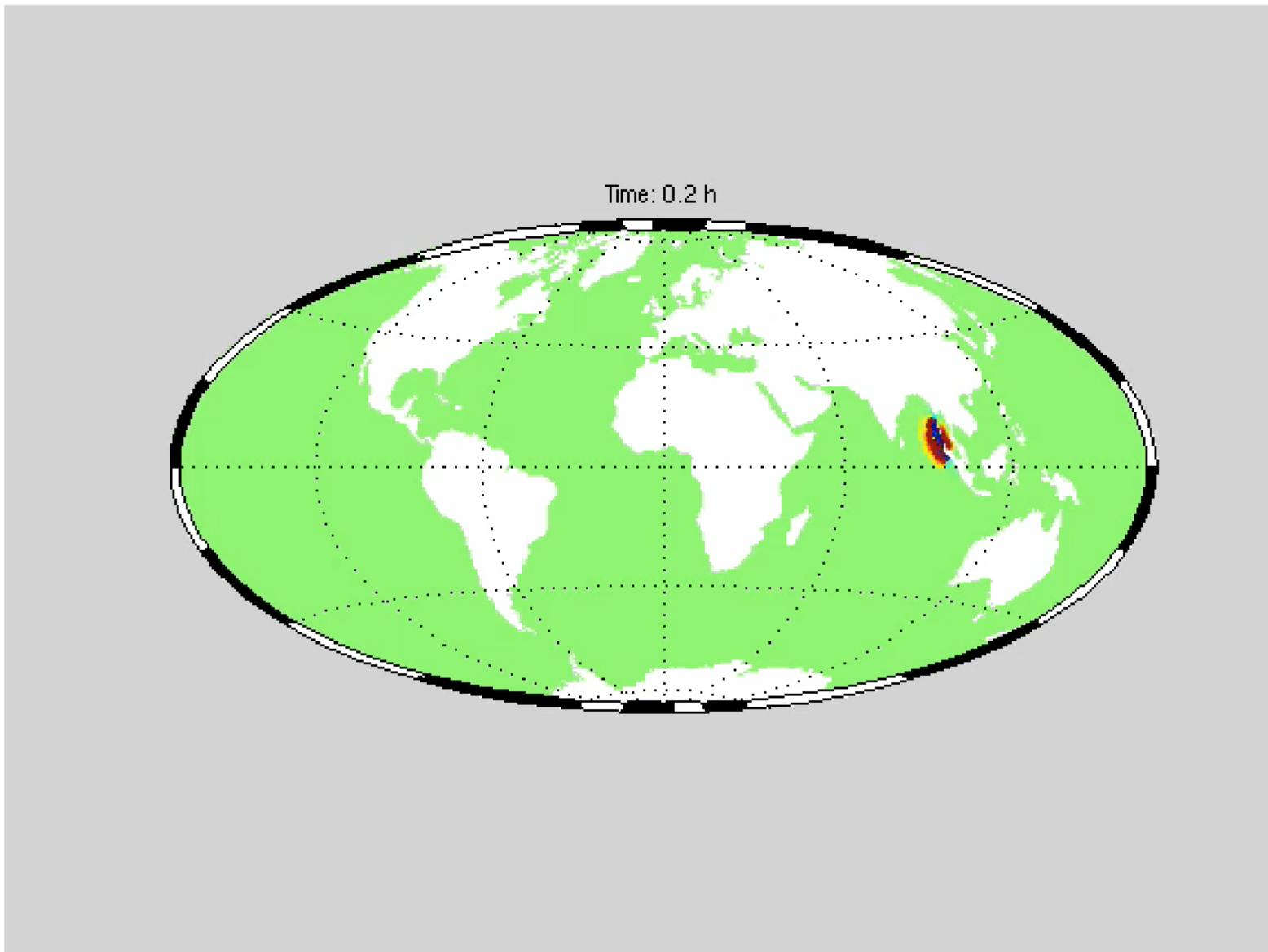
$$\mathbf{v} \cdot \mathbf{n} = \sqrt{\frac{g}{H + \eta}} \eta$$

# *Initial Conditions*

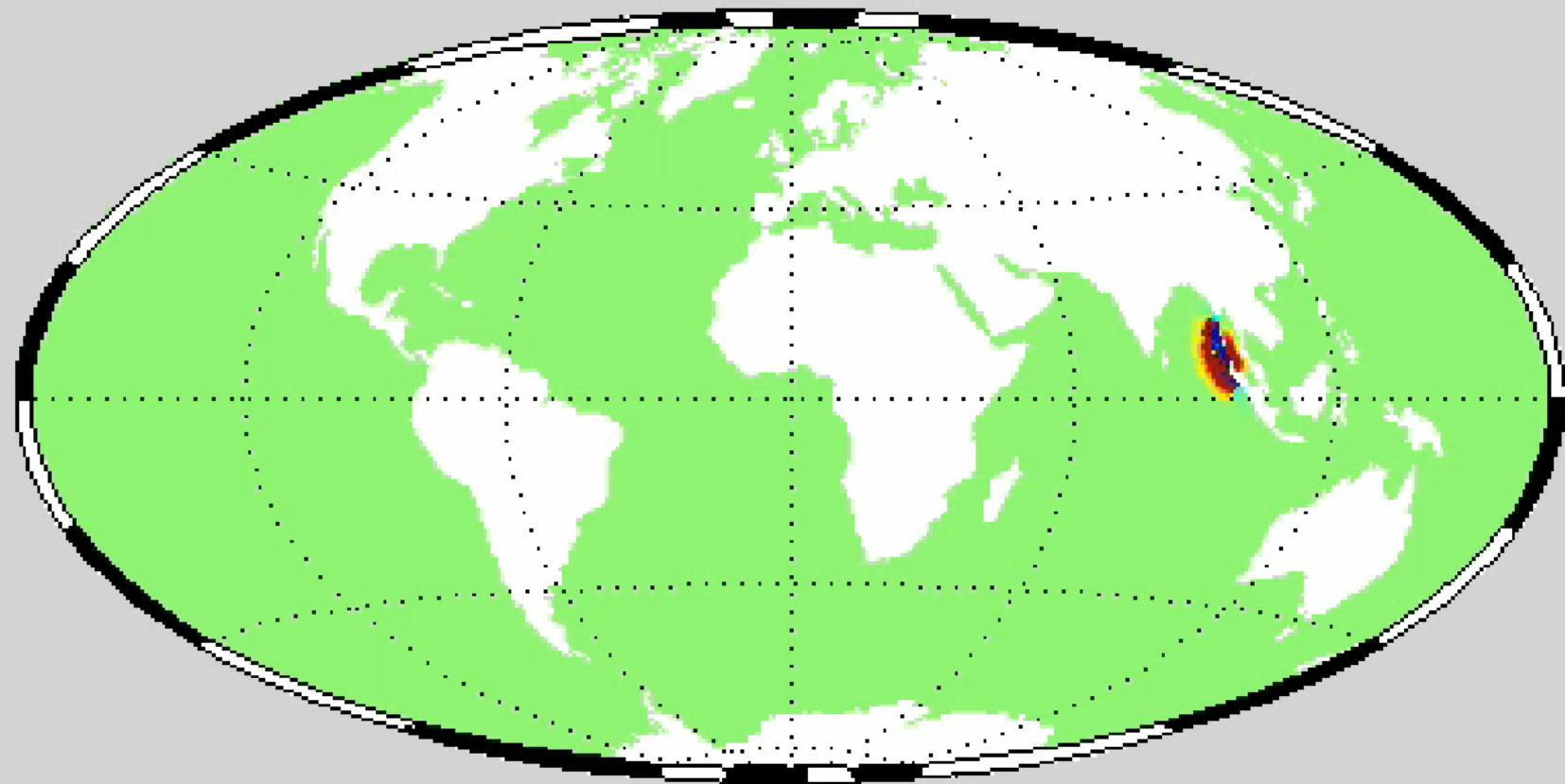
- Simplified
- Okada Plate Model
- Complex



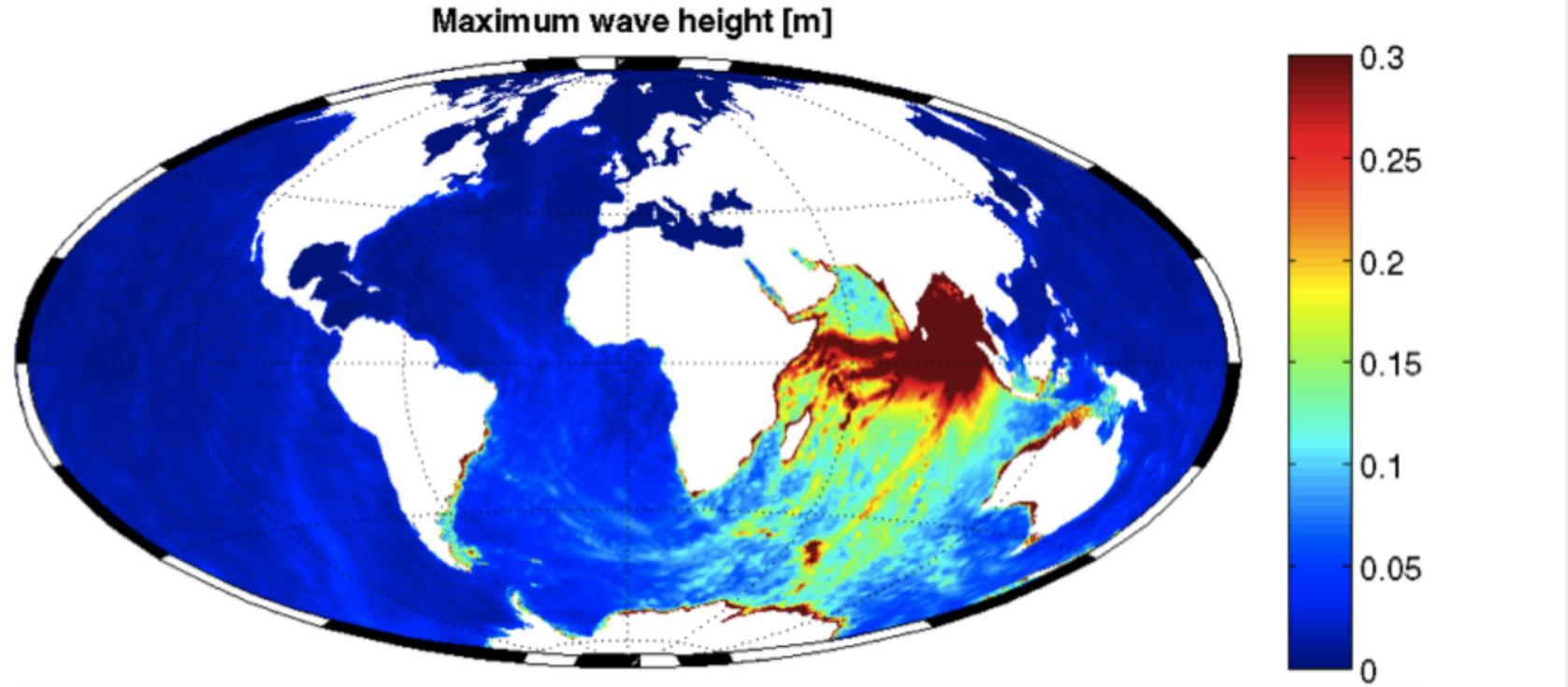
# *Extent*



Time: 0.2 h



# *Multi-Scale Characteristic*

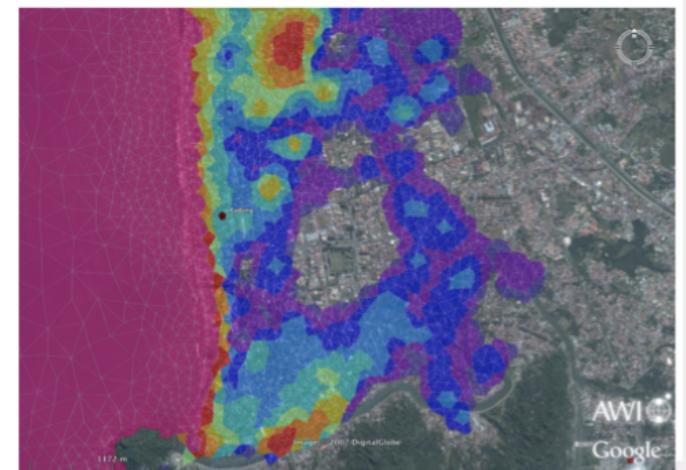


Scales:

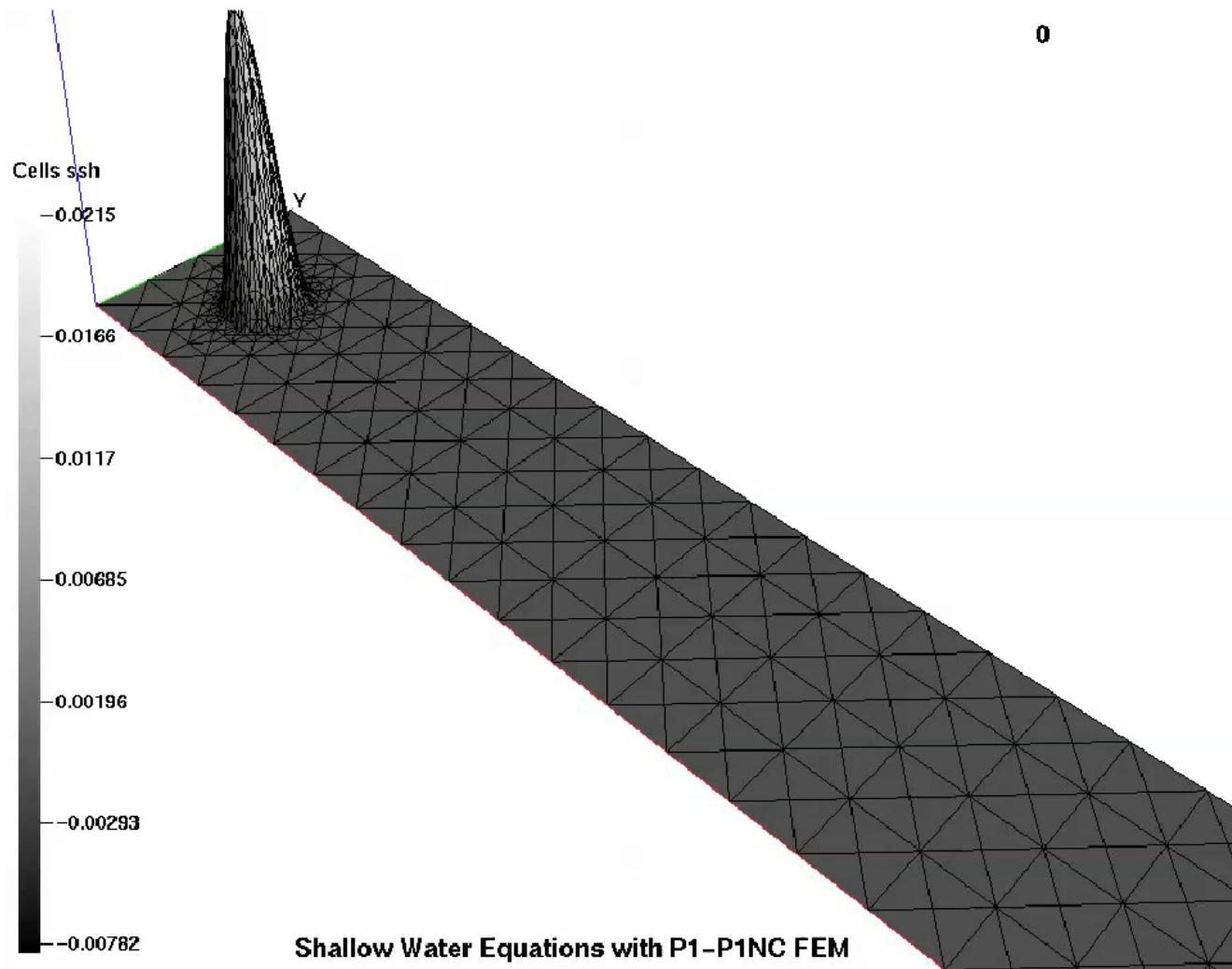
Global:  $\mathcal{O}(10.000\text{km})$

Deep Ocean:  $\mathcal{O}(100\text{km})$

Coastal Inundation:  $\mathcal{O}(0.1\text{km})$



# Adaptive Mesh Modeling



refine if  $\nabla h|_\tau > \theta_{\text{ref}} \max(\nabla h|_\tau)$   
 $\theta_{\text{ref}}$  threshold value

0

Cells ssh

-0.0215

-0.0166

-0.0117

-0.00685

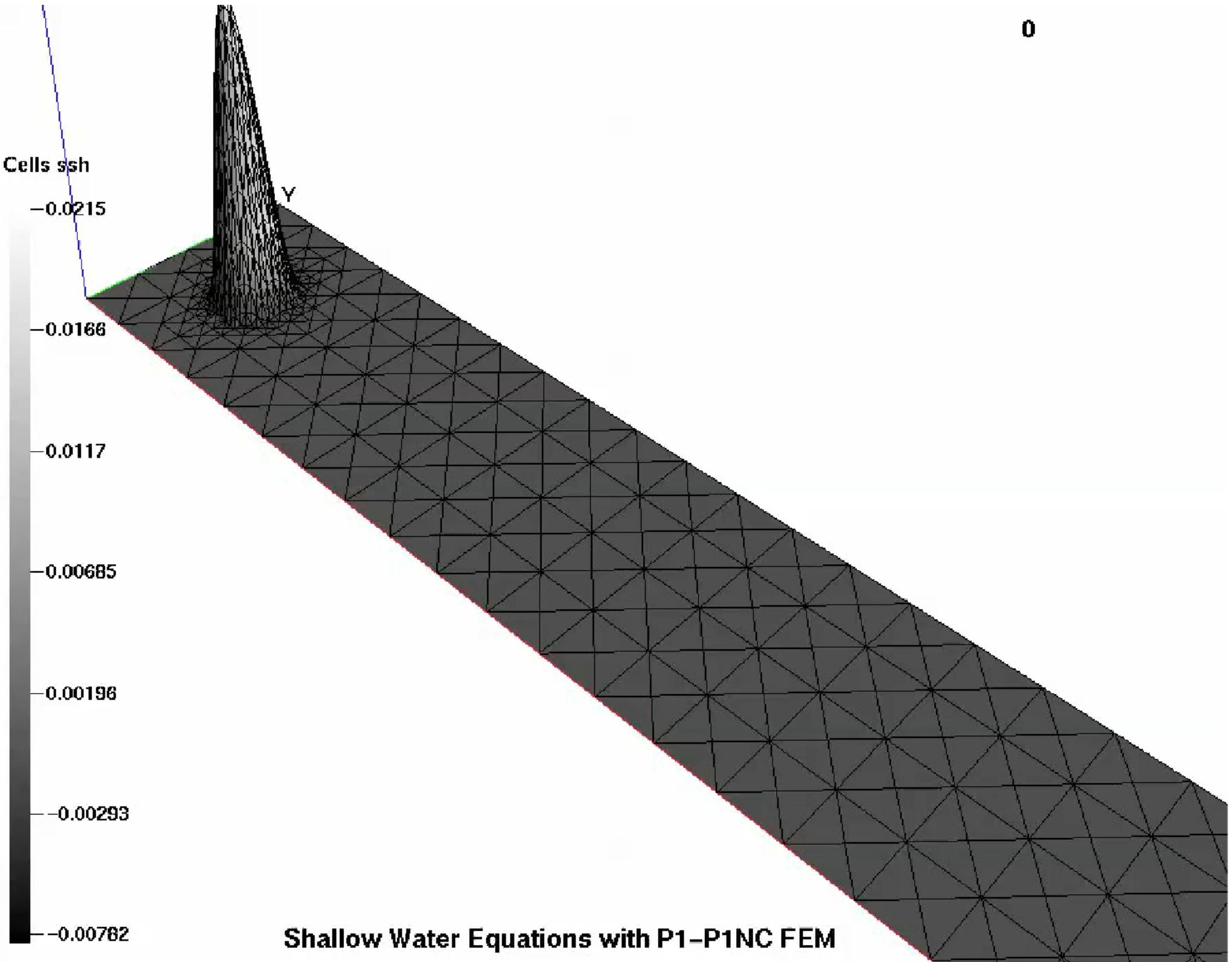
0.00196

-0.00293

-0.00762

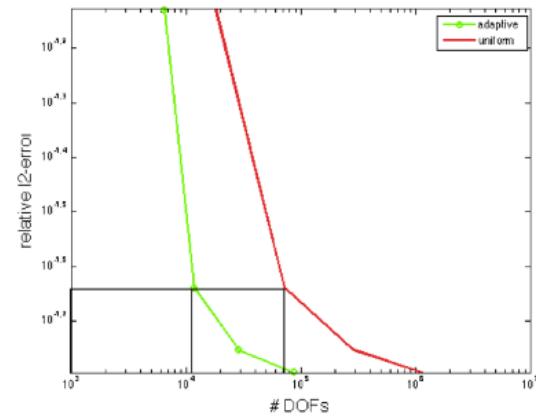
Shallow Water Equations with P1-P1NC FEM

Y



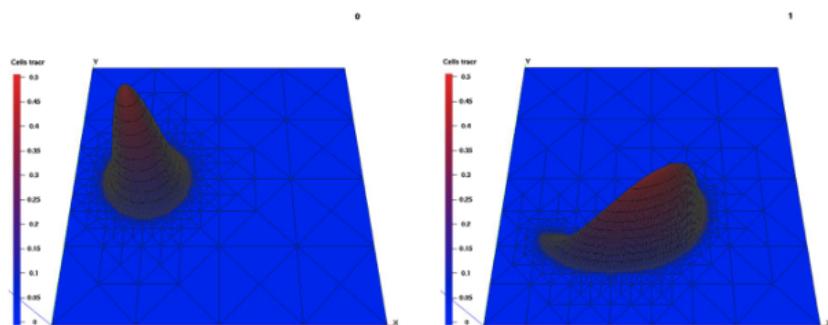
# *Adaptive Mesh Efficiency*

DOFs for given error:

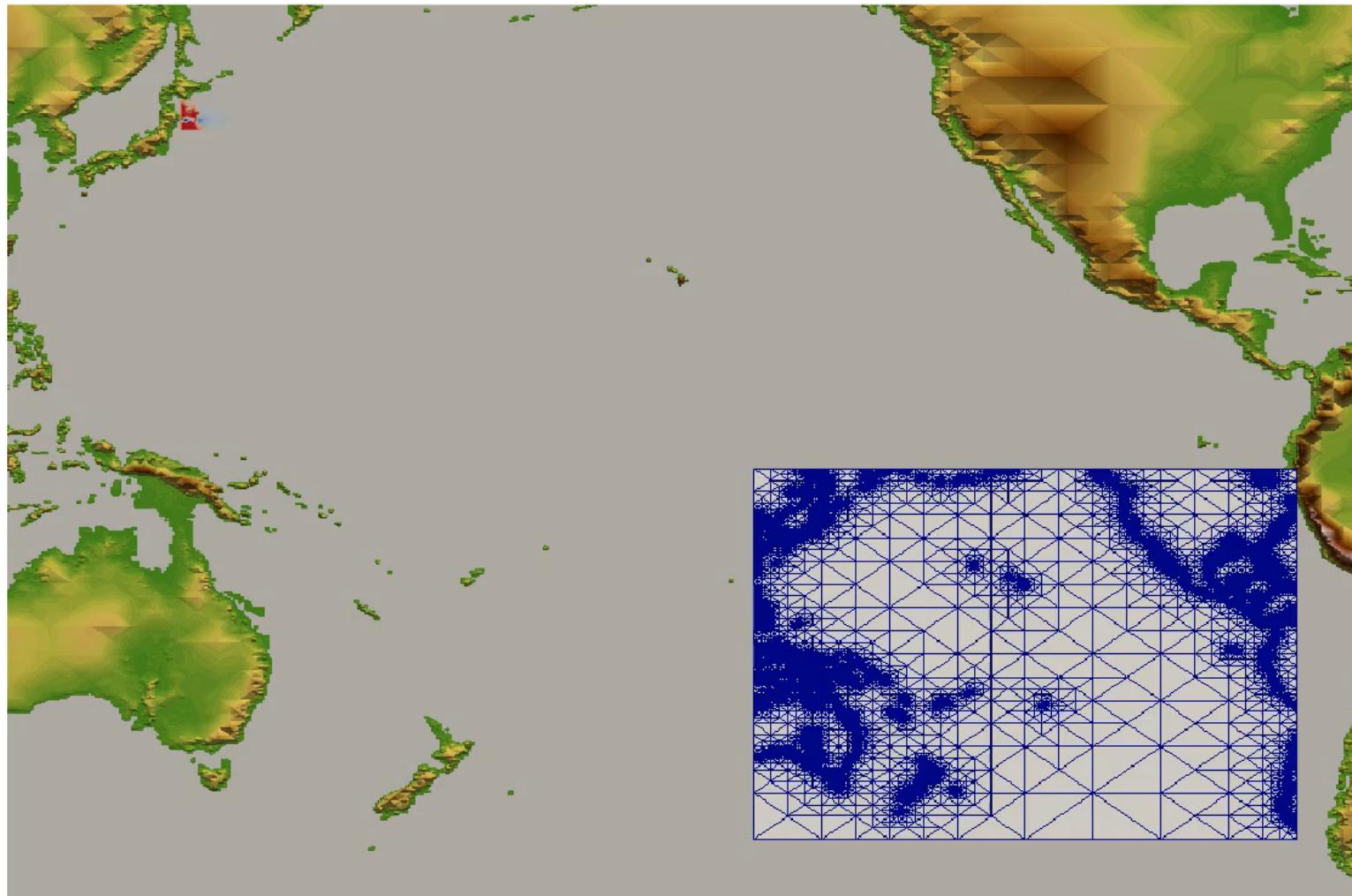


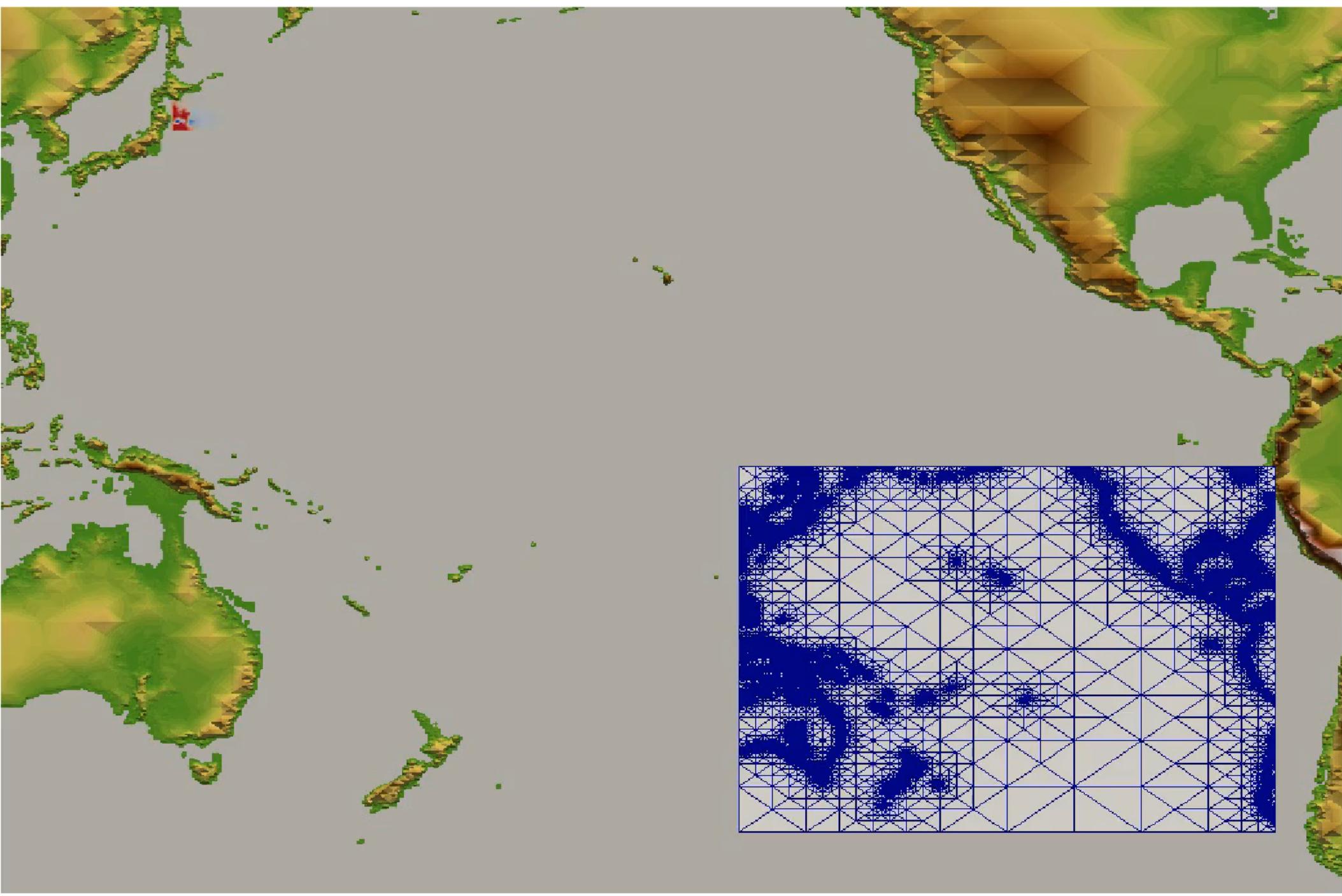
Time for given error:

Error:	$10^{-7}$
Adaptive:	6.1 s (5k nodes)
Uniform:	230.5 s (66k nodes)



# *Tohoku Earthquake/Tsunami*

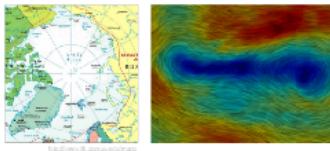




# Example: Adaptive Atmospheric Tracer Simulation

## Problem: Ozone Depletion

Does it take place over Arctic?



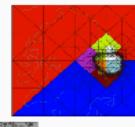
## Situation Description

Does it take place over Arctic?

- High ozone over the entire Arctic!
- Missing hole observed!
- But small areas of ozone depletion
- Significant ozone decrease

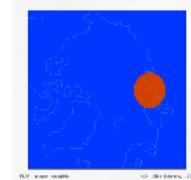
## Optimization with SFC

- Domain decomposition for parallel computation
- Space-filling curve approach
- Dynamic load balancing



## AMR Simulation

- Adaptive Mesh allows local resolution 5 km
- Wind shear leads to filaments!
- There is ozone depletion!



## State-of-the-Art Simulation

- Resolution: 50 km (high for climate application)
- Wind also given with 50 km resolution
- Simplification: 2D (only atmospheric layer)

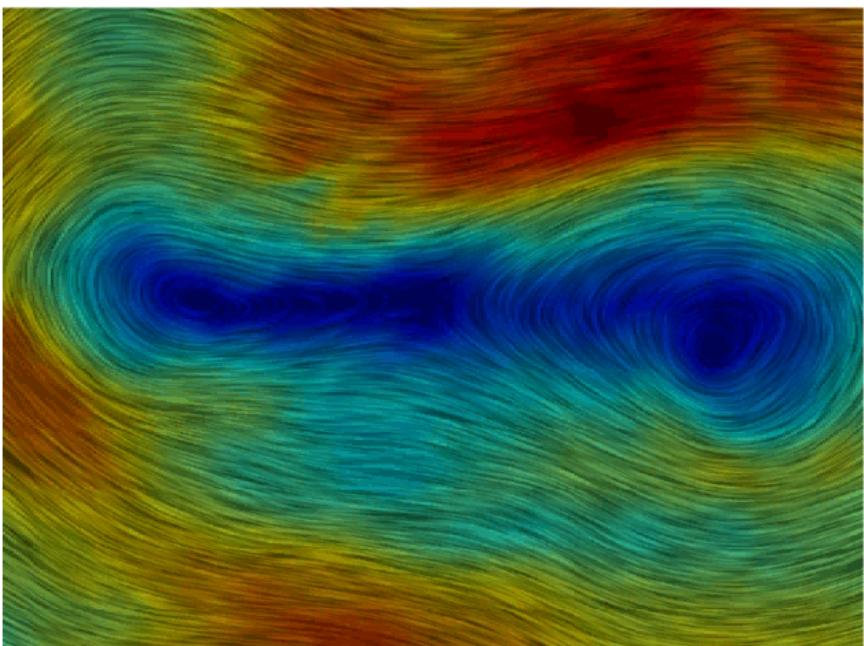


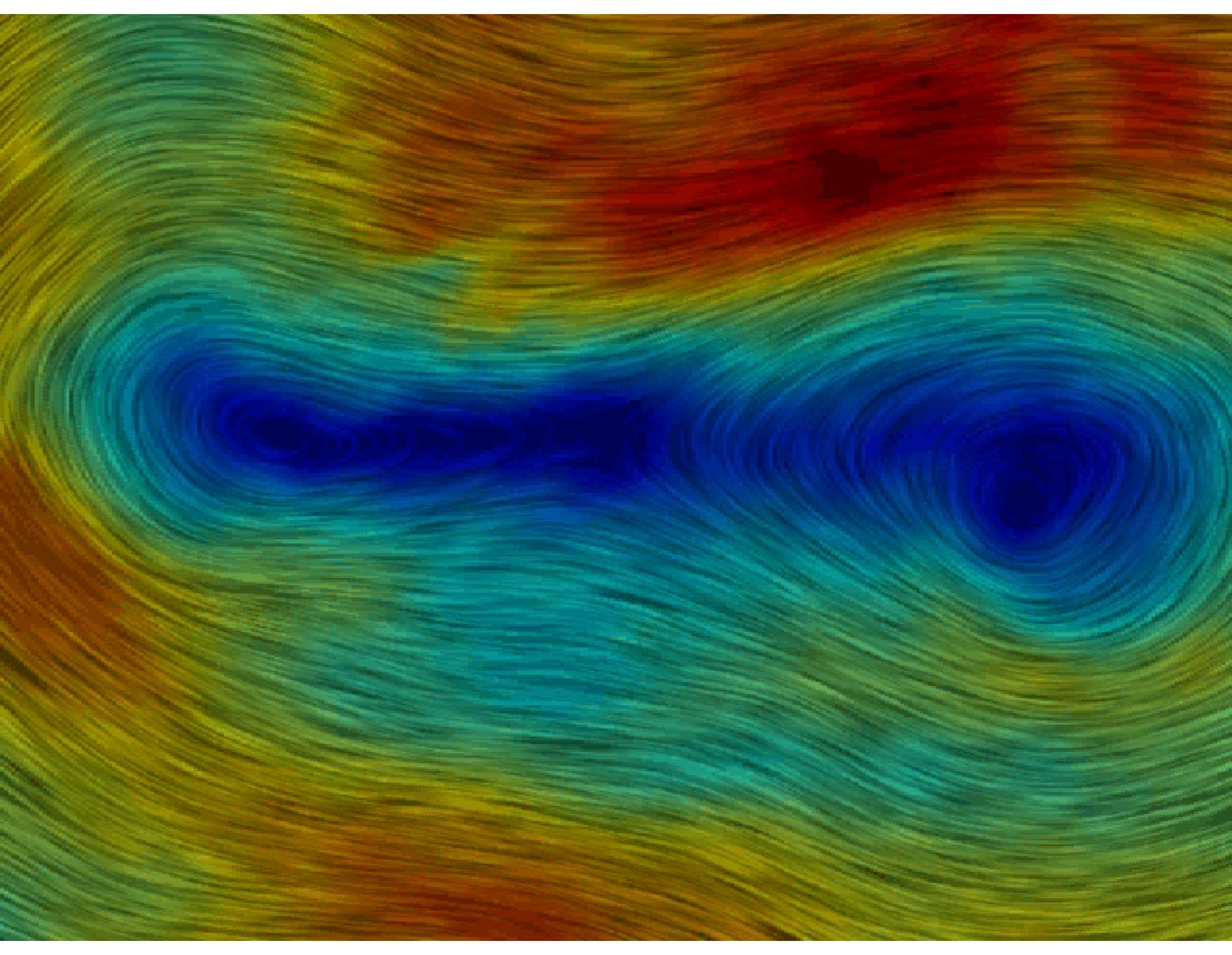
# *Problem: Ozone Depletion*

Does it take place over Arctic?



<http://www.lib.utexas.edu/maps>





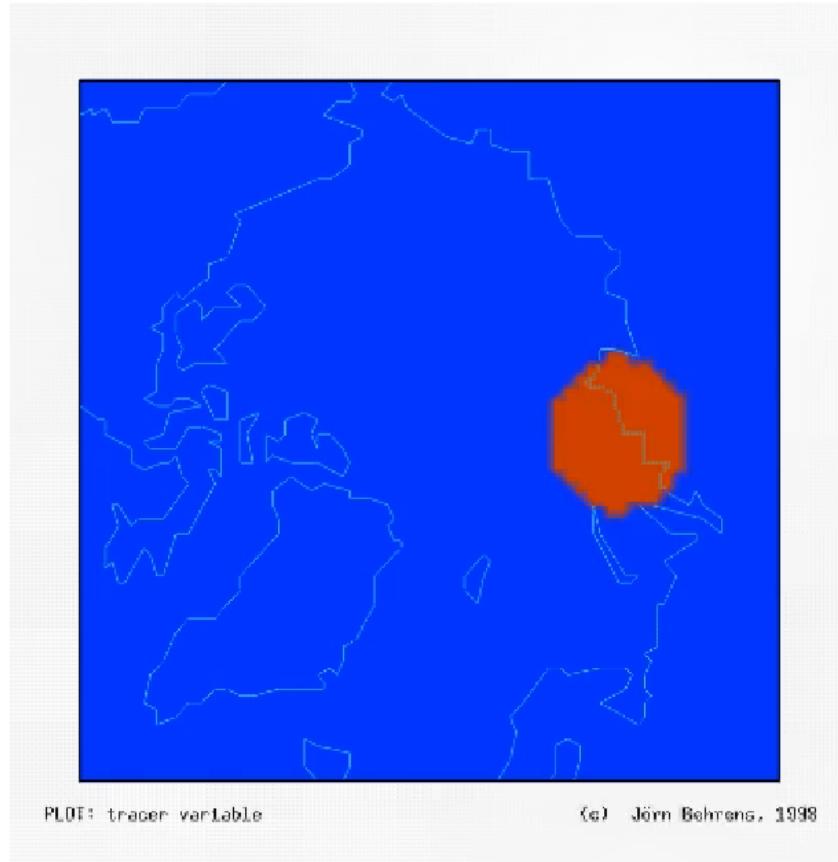
# *Situation Description*

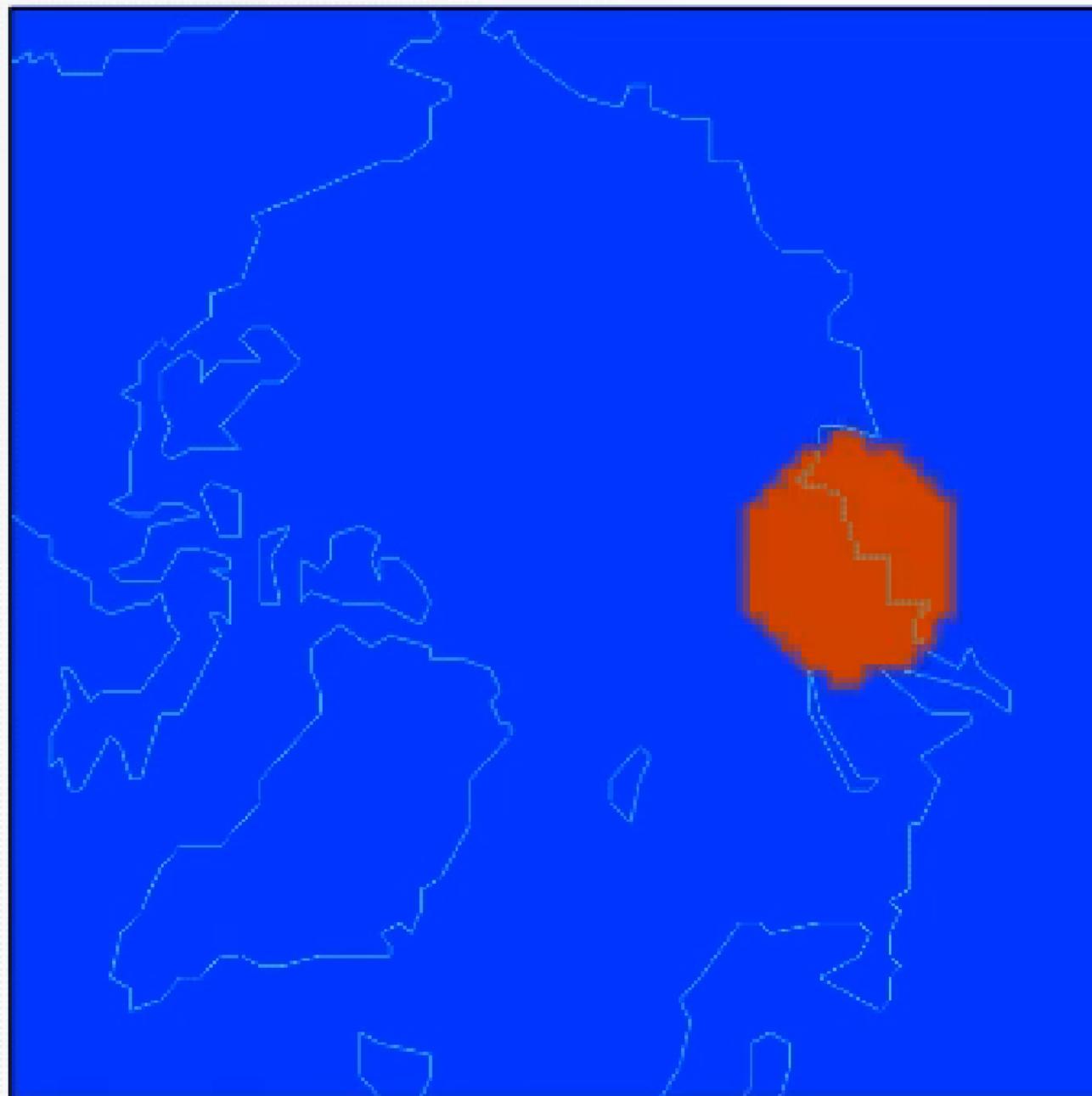
Does it take place over Arctic?

- Physics works the same as Antarctic
- No ozone hole observed
- But small areas of ozone depletion
- Dynamics quite different

# *State-of-the-Art Simulation*

- Resolution: 50 km (high for climate applications)
- Wind also given with 50 km resolution
- Simplification: 2D (only stratospheric layer)



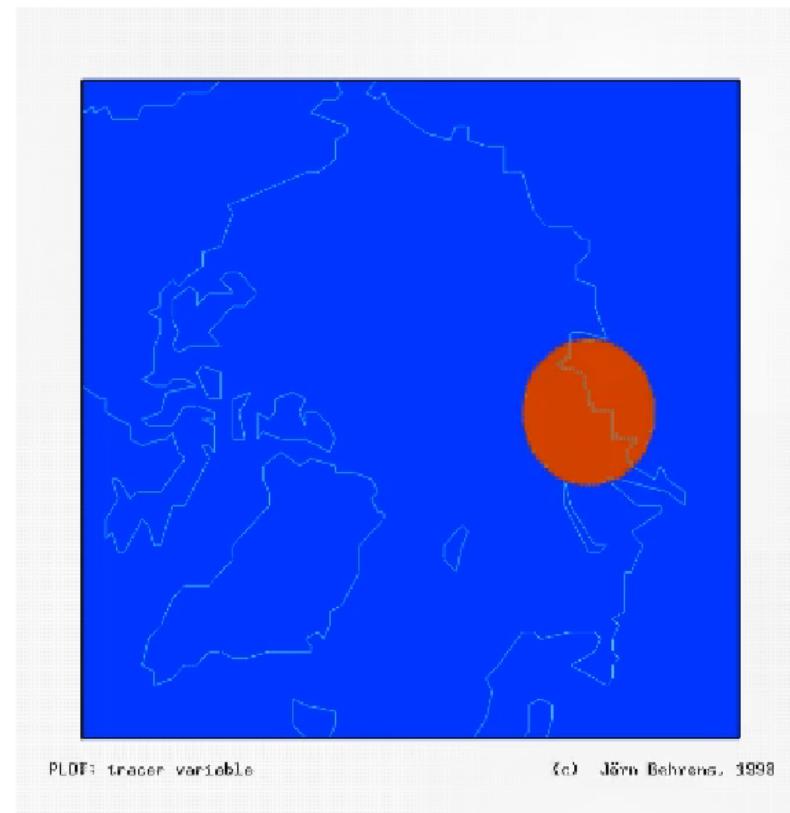


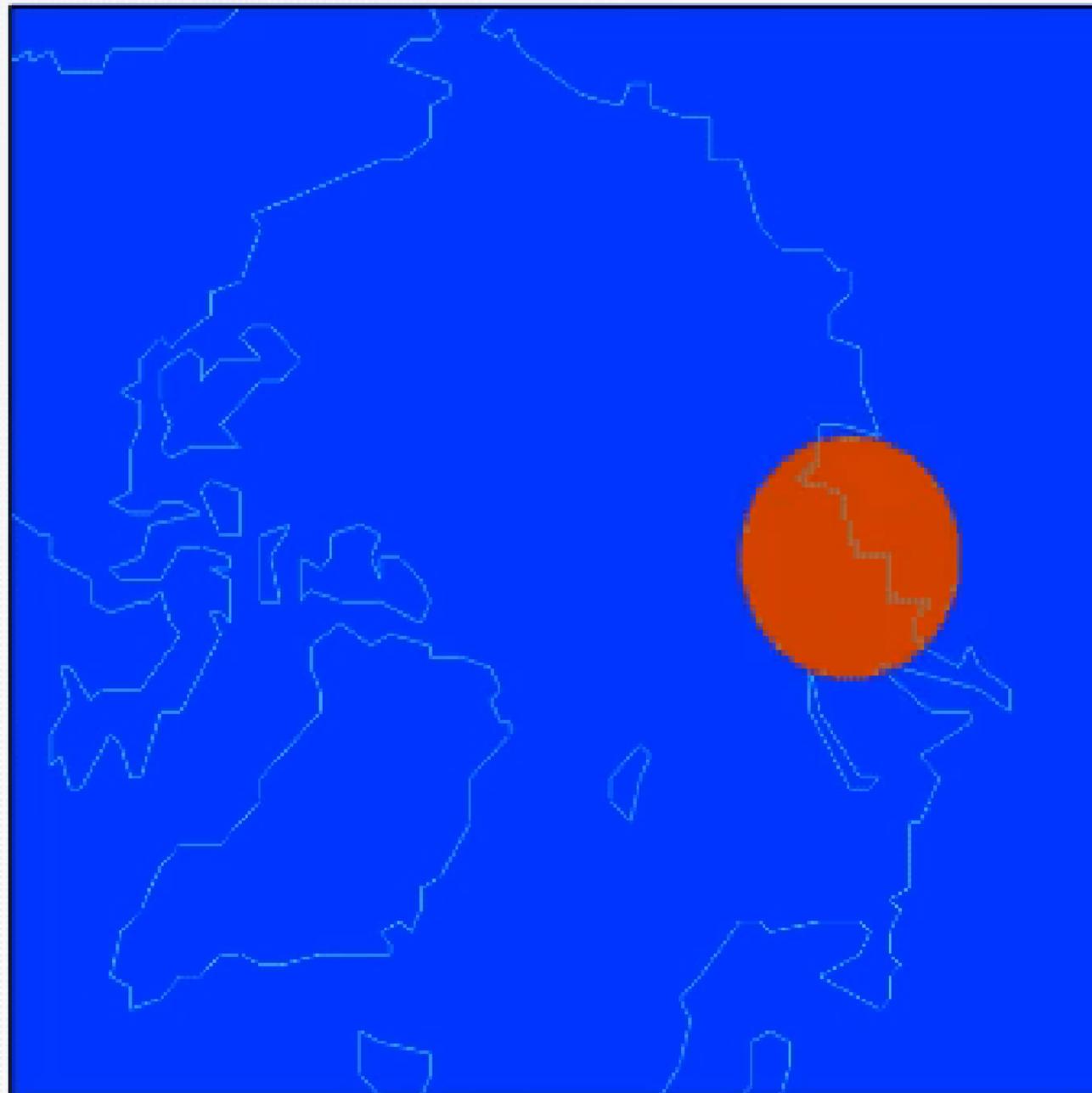
PL0T: tracer variable

(c) Jörn Behrens, 1998

# *AMR Simulation*

- Adaptive Mesh allows local resolution 5 km
- Wind shear leads to filaments!
- There is ozone depletion!



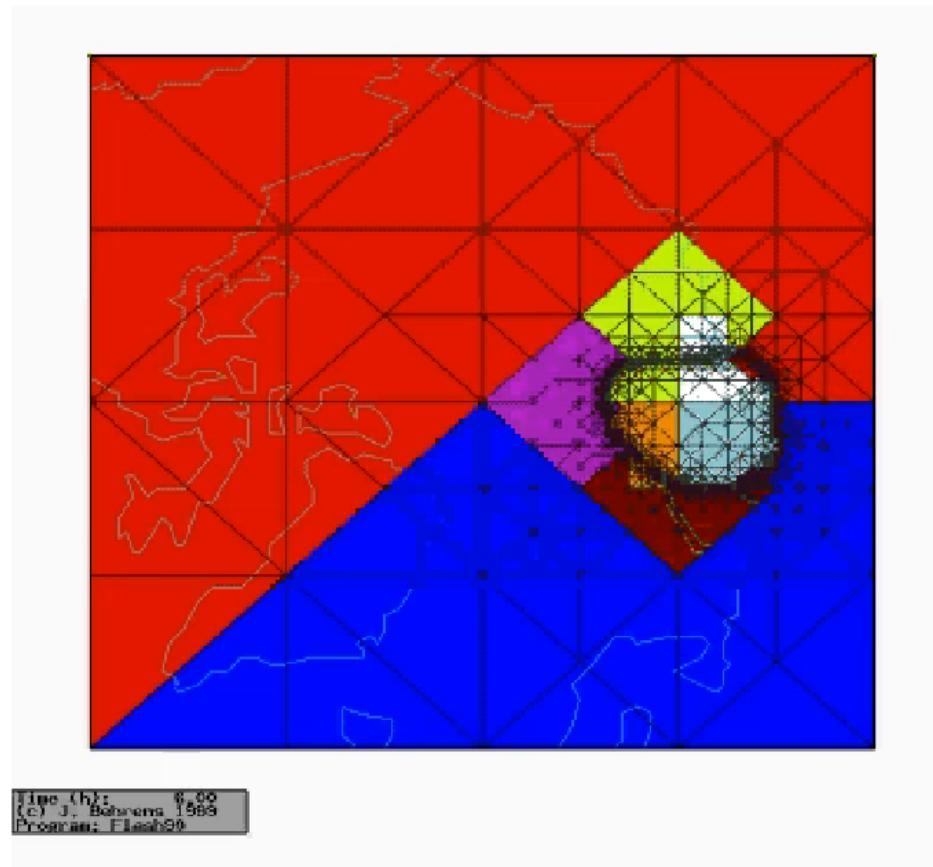


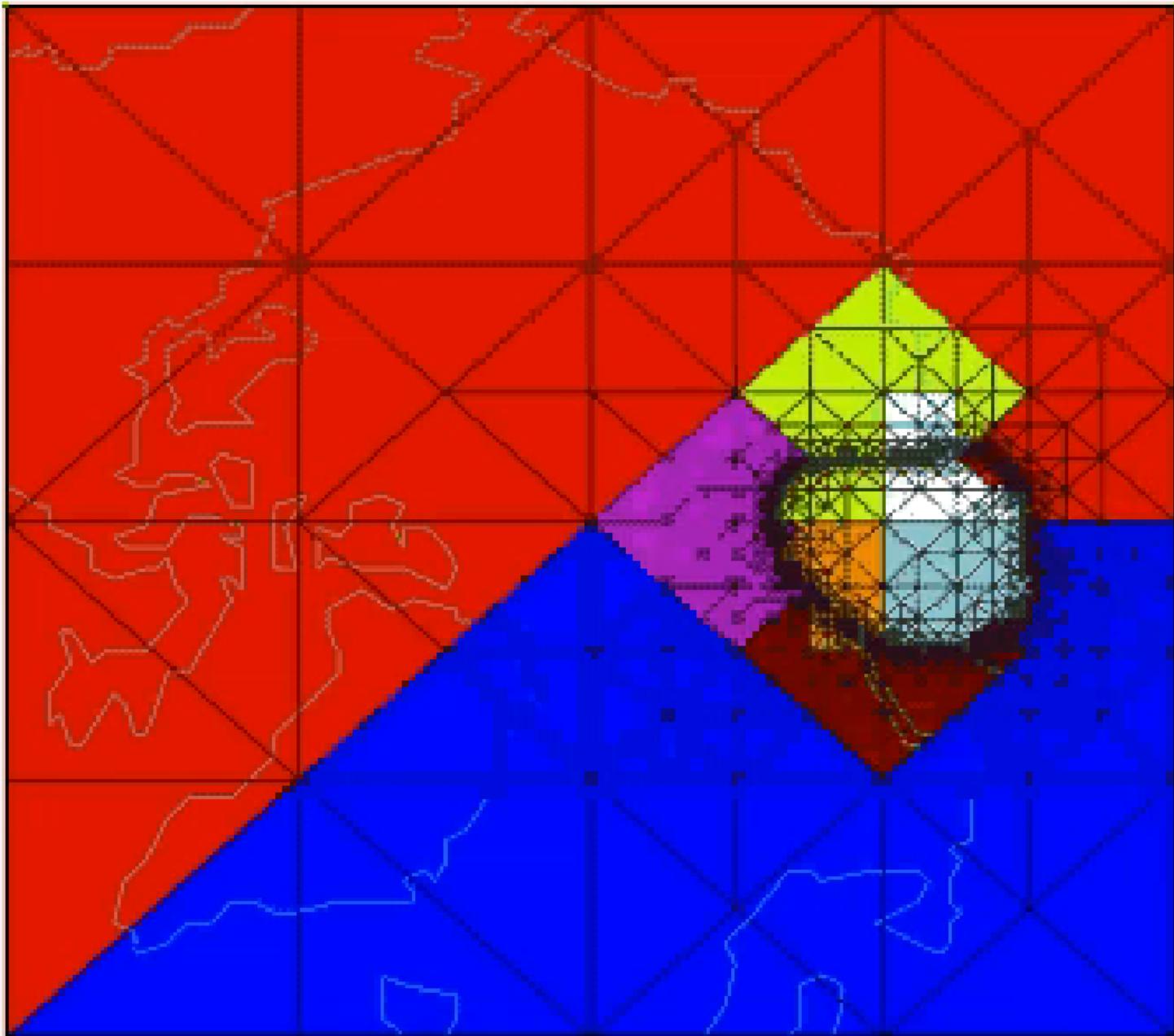
PL0F: tracer variable

(c) Jörn Behrens, 1998

# *Optimization with SFC*

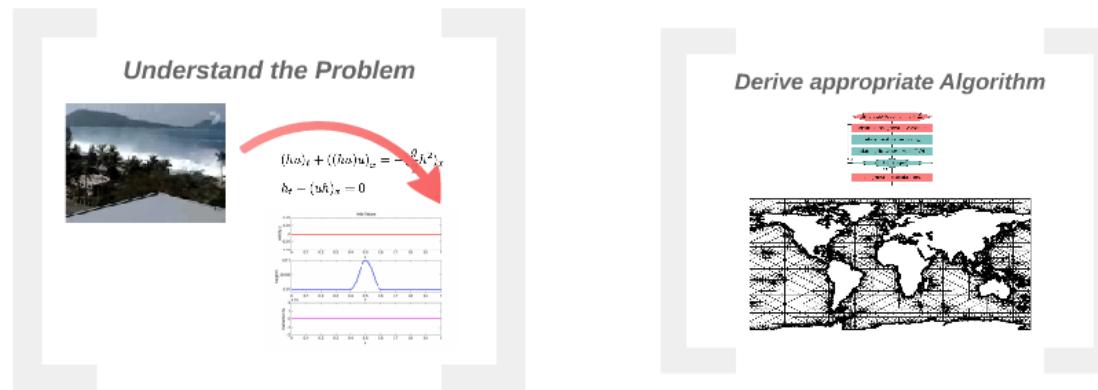
- Domain decomposition for parallel computation
- Space-filling curve approach
- Dynamic load balancing





Time (h): 6.00  
(c) J. Bohren 1999  
Program: Eleoh90

# General Questions of Scientific Computing



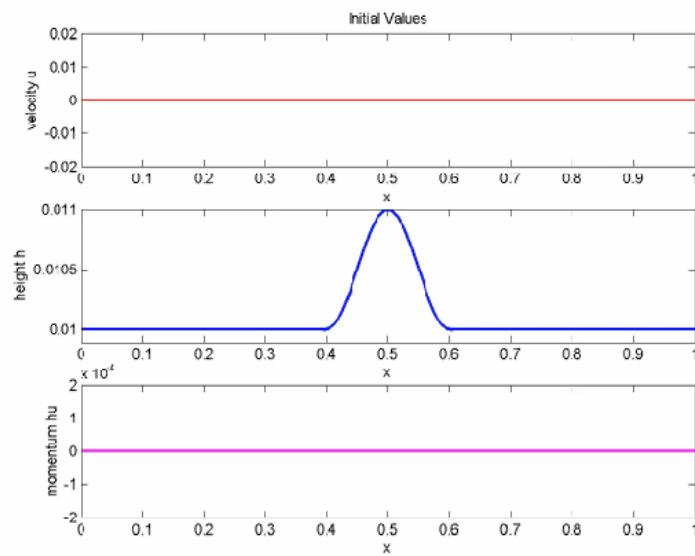
Simple principles of computer architectures



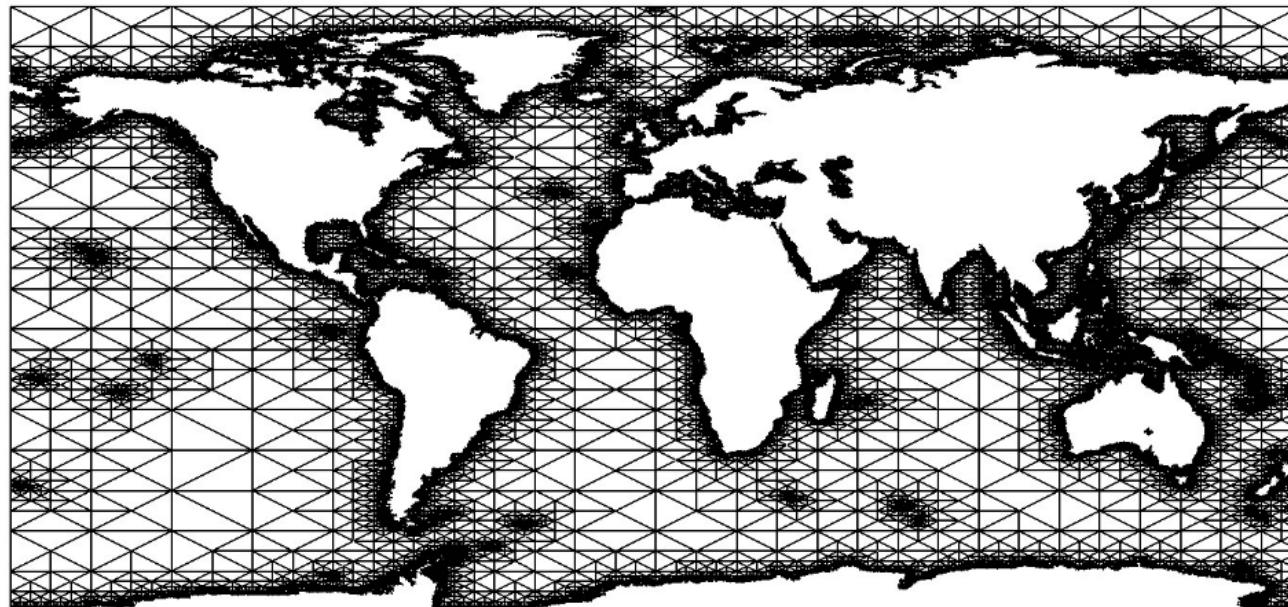
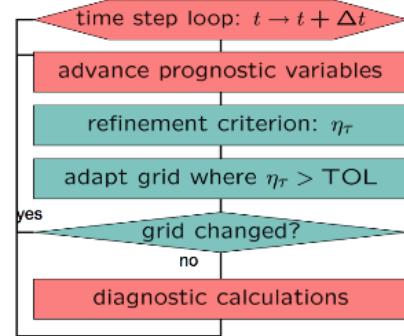
# *Understand the Problem*



$$(hu)_t + ((hu)u)_x = -\left(\frac{g}{2}h^2\right)_x$$
$$h_t + (uh)_x = 0$$



# Derive appropriate Algorithm

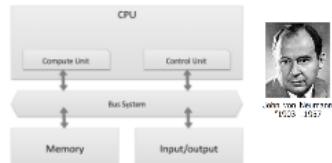


# *Understand the Computer*

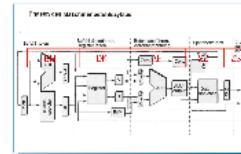


# Simple principles of computer architectures

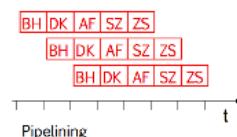
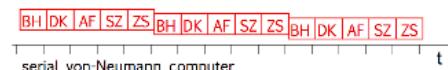
Von Neumann Architecture



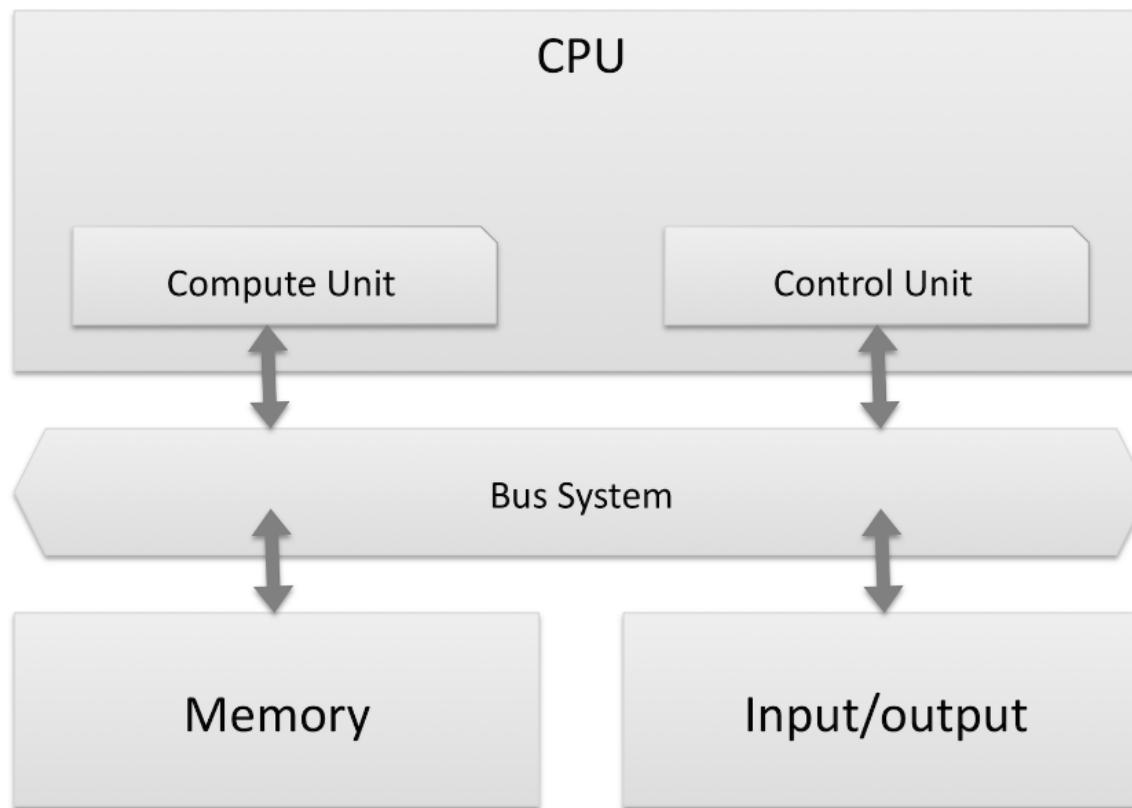
Operation via Instructions



Elements of Acceleration

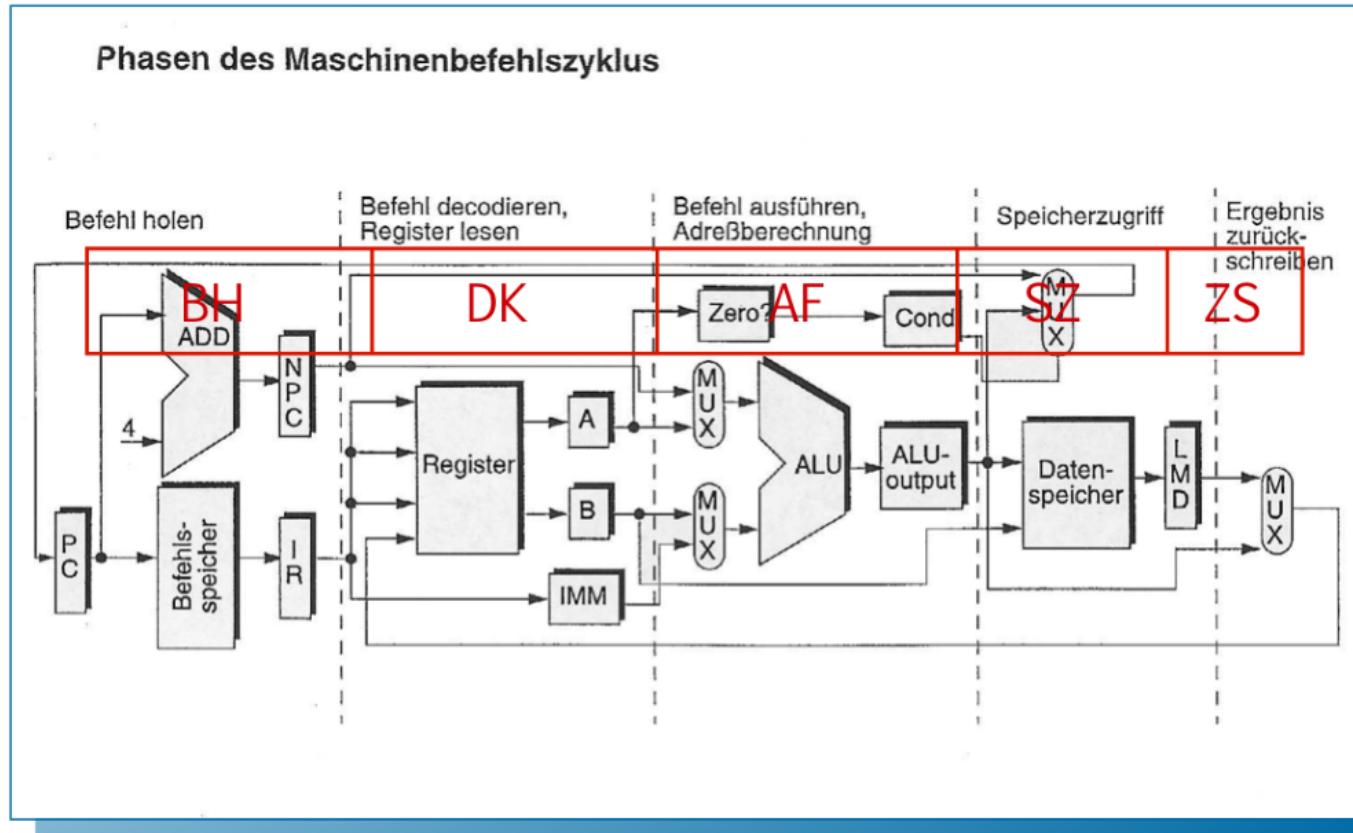


# *Von Neumann Architecture*



John von Neumann  
\*1903 ..1957

# *Operation via Instructions*



# *Elements of Acceleration*

