# MODELING OF LARGE-SCALE SYSTEMS



### K.C. Hansen



# (WHAT DOES THE COMMITTEE REALLY WANT FROM ME?)



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### MODELING OF LARGE-SCALE SYSTEMS (OOPS ... MARGY IS GIVING THAT TALK)



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### MODELING OF LARGE-SCALE SYSTEMS (NO ... XIANZHE IS GIVING THAT TALK ... AND HIS WILL BE BETTER ANYWAY)

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### MODELING OF LARGE-SCALE SYSTEMS (CRAP ... THE ABSTRACT DEADLINE IS TODAY)



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### MODELING OF LARGE-SCALE SYSTEMS (MODELING CHALLENGES AND COMPARISON TO BUILDING AN INSTRUMENT)



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### MODELING OF LARGE-SCALE SYSTEMS (CRAP ... I'M THE VERY LAST TALK ... THEY MUST HAVE HATED MY ABSTRACT)

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# MODELING OF LARGE-SCALE SYSTEMS

(FRAN SAYS ... I PUT YOU THERE BECAUSE YOU SHOW ENTERTAINING MOVIES TO KEEP PEOPLE INTERESTED SO THAT THEY WILL STAY UNTIL THE END)



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### MODELING OF LARGE-SCALE SYSTEMS (MODELING CHALLENGES AND COMPARISON TO BUILDING AN INSTRUMENT)



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University of Michigan Center for Space Environment Modeling

> - and – Modelers Everywhere



 Developing a high quality, large-scale simulation model is comparable in scope to designing and building a spacecraft instrument

 Using these models is similar in complexity to using and interpreting spacecraft data

There are many challenges that must be overcome when developing and running these models

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### Model vs Instrument Development

		Michigan MHD Model BATSRUS/SWMF	MIMI Instrument/Cassini Huygens
	Years (Development)	15	7+7
	Years (Science)	15	9
	Cost (Development/Operatio ns)	~\$20 M	~\$30 M
	Cost (Science)	~\$15 M	~\$10 M
	Development /Operations FTEs	~10	~15
	Objects studied	21	7
		Sun, Mercury, Venus, Earth, Mars, Jupiter, Saturn, Uranus, Io, Europa, Enceladus, Titan, 6+ comets, Heliosphere, Extra-solar star-planet interaction	Jupiter, Saturn, Enceladus, Rhea, Dione, Titan, Heliosphere
	Funded by	NASA/DOD/NSF - Mostly space weather applications	NASA- Cassini/Huygens mission
	Mass	400,000 Lines of code	16 kg
	Wow	~\$50/Line	~\$1.5 M/kg
K.C. Hanser	Required!	Validation	Calibration



### Xianzhe Jia - Profile of a Modeler

ncor."			$\star$ The Modeler $\frown$		
Metric		Value	A 🛨 The Stats		
CPU Hours Used (2010)		~ 1,000,000			
Equiv. number of full time processors		128	X - Lafredrig Table Table		
Annual value of those processors		~\$500,000			
For a Typical run					
	Number of cores	256 - 512			
	CPU Hours	50,000	and the second s		
	Wall time	12-24 hr	100-14 300-14		
	Time in queue	2-48 hr	Xunnhe Jia (Univ. of Michigan) ★ The Model ★ The REALLY large hard drives on the modeler's desk		
	Preparation time	Days			
	Times to try each run before success	2-4			
	Size of output files	1GB per hour simulated			
	Typical number of hours simulated	1000-2000 hr			

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### Multiple Length Scales

□ 2000 R<sub>J</sub> Jupiter's magnetotail (> 4AU)
 □ 100 R<sub>J</sub> Jupiter's bow shock
 □ 1 R<sub>J</sub> Boundary Conditions
 □ 0.5 R<sub>J</sub> Current sheet thickness
 □ .025 R<sub>I</sub> Io's radius

# 2000 R<sub>I</sub> / 0. 025 R<sub>I</sub> = 80,000 $\approx 2^{16} !!!$

### **Options?**

Use 2<sup>16</sup> cells and wait a lifetime for the run to finish
 Develop some kind of non-uniform grid



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#### CFL condition (Courant-Friedrichs-Lewy)





The fastest wave speed

#### Run time in 3D simulations

- $\approx$  #of cells and  $\Delta t$
- <sup>1</sup>/<sub>2</sub> the cell size (double the resolution)
  - 8x more cells
  - $\frac{1}{2}$  the time step
  - Run takes 16 times longer!

#### Square peg in a round hole

- Spherical planets on square grids
- Obvious mismatch
- Hard to get boundaries right
- Hard to resolve scale heights



### **Under-resolved Features and Numerical Errors**

- Numerical discretization results in deviations which mimic physical attributes
  - Resistivity
  - Viscosity
  - Diffusion
- These may not be "wrong" but they are not well characterized and generally cannot be quantified and/or controlled

- Under-resolved Features
  - Are not necessarily "wrong"
  - But ... understanding what is valid and what might not be requires significant experience
  - Will expand until they are resolved (3-5 grid points)
  - Can result in increased transport rates, diffusion rates, ...

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### **Magnetic Fields**



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July 15, 2011



### **Boundary Conditions**

### Overheard at a MOP meeting "What are your boundary conditions?"

- Boundary conditions can control everything in a simulation!
- Wave reflections
- Whether or not magnetic field penetrates a body
- How plasma behaves at a surface
- Including and ionosphere



**Figure 1.** A cartoon showing the three boundaries in the simulation: (1) the core boundary (green circle), (2) the inner boundary (yellow circle), and (3) the outer boundary (black circle).

Credit: Jia, 2009

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# CSEM

cat

## Physics (the good, the bad and the missing) - I

The reality is that ALL models do some things **CORRECT** and some things with **LIMITED** or **NO** fidelity. A realistic consequence of this is:

- Run the model, see what happens
- Be realistic under resolving the system, numerical limits, or leaving out some physics doesn't necessarily invalidate the results. However, you must understand the model's limitation and put results in the proper context
- Just like with data don't misuse, over interpret, ignore limits
- MHD
  - Does better than is should in most applications
  - Numerical resistivity, viscosity and diffusion mimic physical features, but are very difficult to quantify and/or control
- Source terms
  - A simple way to include non-MHD effects
    - Mass loading, momentum loading, charge-exchange, heating, "friction", ...
  - Not described by CFL condition so can make solutions "stiff" meaning more difficult to solve and require smaller time steps
  - Can be hugely important but do not really solve the problem of missing physics





### Physics (the good, the bad and the missing) - II

#### MHD extensions

- Including physics resistivity, viscosity, diffusion
- Multi-species, Multi-fluid (electrons, ions, dust, ...)
- Hall-MHD, conductance models
- Hybrid
- Coupled Models



### Coupling a Ring Current Model to MHD



- For Earth: The SWMF already couples MHD with Ring Current (RCM or HEIDI)
- HEIDI solves the time-dependent, gyration- and bounce-averaged kinetic equation for the phase- space density f(t, R, φ, E, μ<sub>0</sub>)
- Collisionless drifts, energy loss and pitch angle scattering due to Coulomb collisions with the thermal plasma, charge exchange loss with the hydrogen geocorona, and precipitative loss to the upper atmosphere.
- For Earth, the source term for the phase space density calculated by HEIDI is the outer simulation boundary, where particle fluxes must be specified. These fluxes are specified from GM.
  - The numerical work was done to make the coupling work for the Earth. For Saturn we need to modify the source and loss terms and the boundary conditions followed by extensive validation.



our MHD model

### **Coupled HEIDI-MHD Results: Earth**





Comparison of HEIDI and HENA ENA images

12/377

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### Massively Parallel Processing and Message Passing

 Porting a code to a supercomputer to run in parallel is a time-consuming task requiring detailed analysis of the codes features

- Fluid based models, as well as any model calculating a selfconsistent magnetic field, requires frequent communication between processors
- Distribution of cells to processors needs to be carefully optimized in order to minimize message passing time

Hilbert space filling curve. BATSRUS uses this to optimize the cell distribution and message passing

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### **Plasmoids at Saturn**







Credit: Winglee, this meeting.

- Terabytes of information
- Inherently 3D data
- Qualitative and visually appealing vs. quantitative
  - Color vs. lines
  - General vs. extracted along spacecraft track
  - "MHD variables" vs. "instrument"
- Time dependence
- The ability to slice and dice

Can you see me now

### So you have a code ...



- How long will it take to get an account?
- Will I have to be fingerprinted?
- Will my non-US-resident graduate student be able to get an account?
- The machine has a different compiler, will the code even run?
- How long are you willing to wait for the run to finish? A nearly universal constant!
- The typical trade-offs
  - Resolution vs. time
  - Physics vs. time

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### "Data" Requires "Modeling" Also

- Forward modeling of CAPS singles data by Rob Wilson
- Data: 2004-2009
  - 3-4 minute intervals
  - 13,513 intervals
  - 2k 20k iterations of the model for each moment calculation
  - ~1000 hours of data
- ~5000 processor hours to compute the moments
- Take home message: some data is highly processed and dependent on the processing method and its built in assumptions



### Models vs Instruments

	Models	Instruments
Unknowns	Discretization effects Missing physics	System "drivers" "time" vs. "spatial"
It's NEW, but is it REAL?	Numerical artifacts Interpretation takes skill	Instrumental artifacts Interpretation takes skill
Assumptions	Physics Parameters (knobs)	Outside FOV Instrument behavior Raw vs. processed
Basic unit $\rightarrow$ processing $\rightarrow$ desired unit (as an example)	Moments $\rightarrow$ Counts	Counts $\rightarrow$ Moments
It all boils down to!	Tightly control inputs Ability to "Experiment"	"Ground truth" Motivation

### We all need each other!

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Go MOP!

Credits:

Saturn

Jupiter

Uranus

Titan

Enceladus

Ganymede

Io







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### Modeling Issues

- Multiple Length Scales <> Grid requirements
- Resolution <> time step + compute time
- Round planets <> square grids
- What happens when you under-resolve
  - Example from Peter Delemere
- Source Terms <> CFL condition issues
- Alfven speed <> time step
  - Strong magnetic fields cause all kinds of problems
  - Hybrid ... whistler ... even worse!
- □ Conservation! (of density, energy, ...)
- Boundary conditions!!!
- Visualization

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- Example from Robert Winglee
- Physics (The good, the bad and the missing)
  - MHD/Fluid
    - Straight up MHD
    - Multi species
    - Multi fluid
    - Hall
    - Plasma + neutrals
    - Semi-relativistic
    - .
  - Hybrid
  - Coupling to include additional physics
  - Assumptions
    - Neutral densities
    - Sources
- Doing Runs
  - Finding a big enough computer
  - How long are you willing to wait
  - Beating the queuing system
  - \$Cost
  - Compromises
    - Resolution <> time



### Model <> Instrument Development

- Heritage (family trees)
- Where did the code/instruments start
- Branches how many versions are there now
- Version control
- Development
  - Time
  - Manpower
  - Cost
- Validation <> Calibration
- Algorithm <> Technology development
- Unknowns
  - Drivers
  - Instruments
    - Internal vs. external
    - Time variation vs. spatial variation
    - Calibration / other instrument parameters
  - Models
    - Missing physics
    - Effect of grids, method, ...
  - What you do when you get the data
    - Is it real?
      - Numerical artifact vs. physics
      - Instrument artifact vs. physics
    - Processing and assumptions
      - MHD (moments) -> instrument
      - Instrument (counts) -> distributions -> moments
- What it all boils down to
  - Instruments: "ground truth"
  - Models: the ability to tightly control drivers and to "experiment"
  - We all need each other

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