Numerical space weather forecasting

A Pulkkinen, NASA GSFC

Numerical modeling

- In this class we will discuss more in detail how numerical modeling of space weather phenomena works.
- We will discuss both *empirical models* that have historically played main role in space weather modeling and *first-principles models* that are the ultimate way to model space weather (and any other natural) phenomena.

Numerical modeling

- Although also forecaster intuition/experience plays an important role, we need models for doing actual space weather predictions.

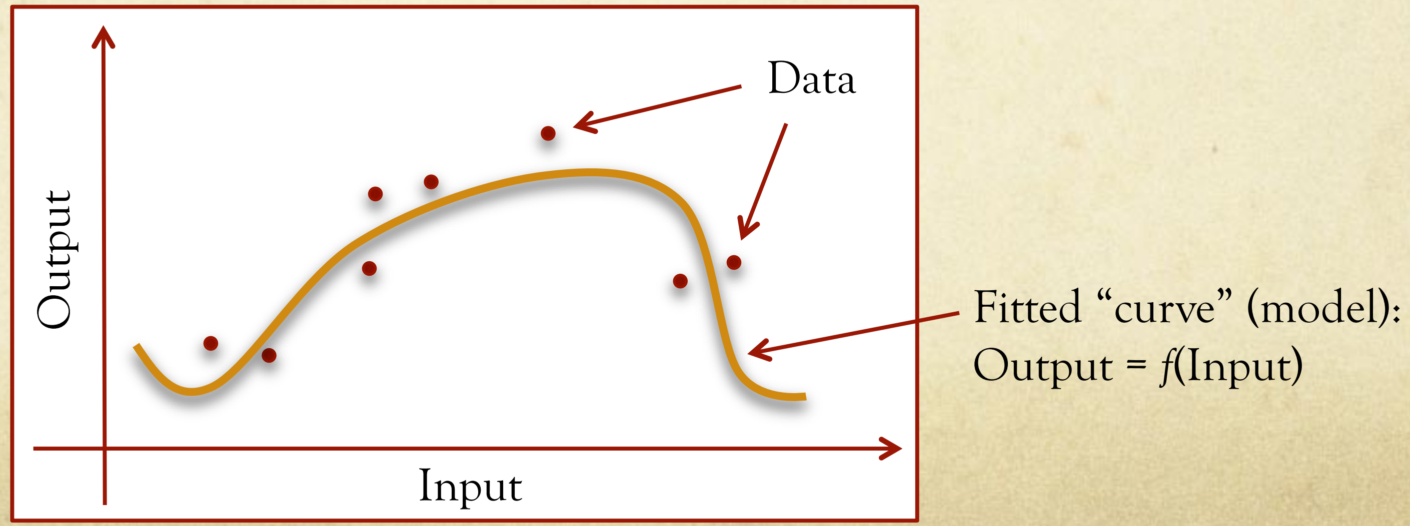
- Models can be divided roughly into two categories:
  - *Empirical models* built directly from observations.
  - *First-principles models* (called also *physics-based models*) built using knowledge about the elementary physics of the system.

- Also *semi-empirical* models blending the two approaches exist.

- The next three slides we discuss empirical modeling but in this class we will focus on the first-principles models.

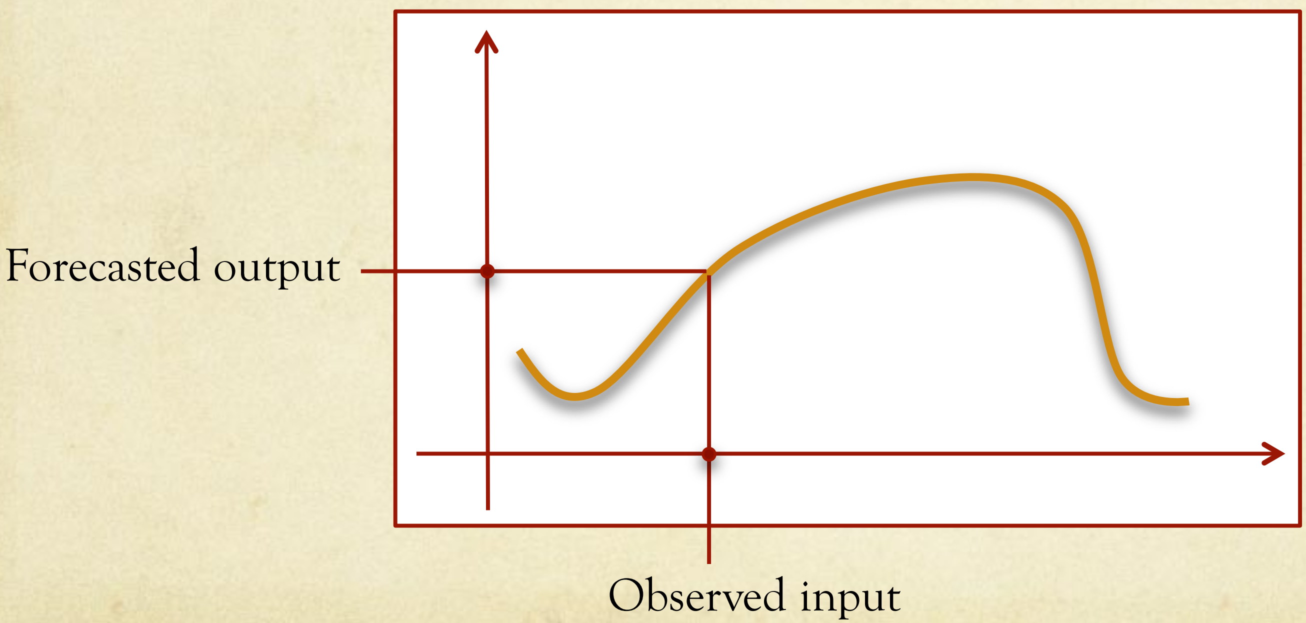
Numerical modeling

- In empirical modeling observations are used build a model that describes the behavior of the system.
- Empirical modeling is essentially fitting a curve (or more generally, function – sometimes a very complicated one) to the input-output data. Input-output data often multidimensional.



Numerical modeling

- The fitted “curve” is then used to forecast new output from the known input.



Numerical modeling

- Because the models are fitted to observed data, empirical approach is very tough to beat for modeling average conditions.
- However, empirical models do not necessarily extrapolate well to extreme conditions not “seen” by the observed data.
- iSWA has a number of empirical models that are useful for forecasting purpose.

Numerical modeling

- In physics we describe the evolution of the system using mathematical equations. Calculus the standard language used to express these equations.

- For example, simple harmonic oscillator is described as:

$$m\frac{d^2x}{dt^2} = -kx \qquad (1a)$$

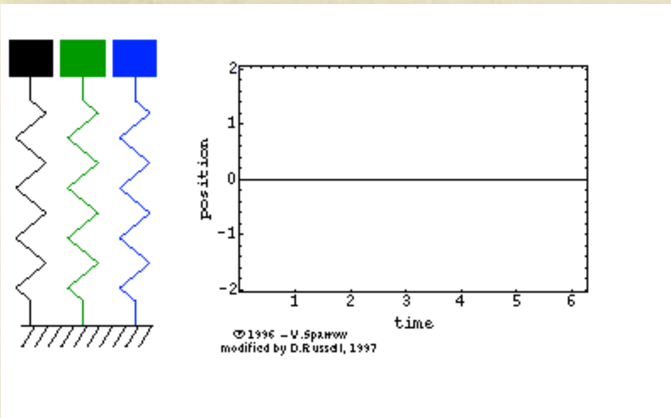
with *analytical solution*

$$x(t) = A\cos(\underbrace{\omega}_{\sqrt{k/m}} t + \phi) \qquad (1b)$$

From initial conditions

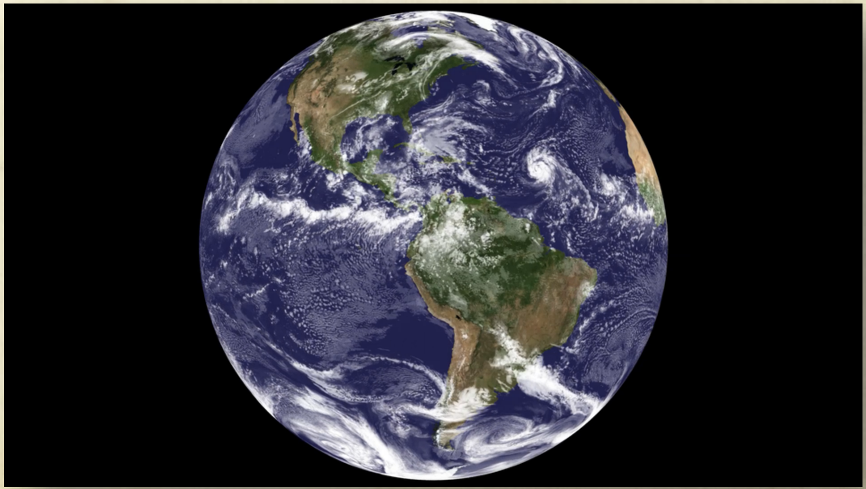
Numerical modeling

- Unfortunately analytical solutions are available only for a fairly small number of physical situations of interest.
- Analytical solutions generally not available for dynamic spatiotemporally extended nonlinear natural systems such as weather or space weather.



Harmonic oscillators (credit: Penn State University)

versus



Clouds from a simulation using the Goddard Earth Observing System Model Version 5 (credit: NASA GSFC SVS)

Numerical modeling

- When analytical solutions are not available one needs *numerical modeling/numerical simulations* for studying the physical system of interest.

- In numerical modeling we use computers to solve the set of equations describing the system.

- Numerical modeling … ingredients:
    - Selection of the system of equations.
    - Selection of the geometry and *numerical grid*.
    - Selection of the *boundary and initial conditions*.
    - Selection of the *numerical scheme*.

We will use modern global geospace MHD modeling to demonstrate these

Numerical modeling

- The first step is to select the equations that capture the key physics of the system of interest.
- One cannot capture and model all physics so one needs to find appropriate approximations containing central physics of interest.
- For example, one cannot model the movement all charged particles and evolution of associated electromagnetic fields in global plasmas: single-fluid *magnetohydrodynamic* (MHD) approach a common approximation.
  - Valid only if the timescales of the physics of interest larger than ion gyrofrequency and the spatial scales larger than ion gyroradius.

Numerical modeling

- The basic set of MHD equations in a *conservative form* is:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad (2a)$$

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} = -\nabla \cdot \{\rho \boldsymbol{v}\boldsymbol{v} + \underline{\underline{I}}(p + \frac{B^2}{2}) - \boldsymbol{B}\boldsymbol{B}\} \qquad (2b)$$

$$\frac{\partial U}{\partial t} = -\nabla \cdot \{(U + p)\boldsymbol{v} + \boldsymbol{E} \times \boldsymbol{B}\} \qquad (2c)$$

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E} \qquad (2d)$$

$$\nabla \cdot \boldsymbol{B} = 0 \qquad (2e)$$

$$\boldsymbol{E} = -\boldsymbol{v} \times \boldsymbol{B} + \eta \boldsymbol{j} \qquad (2f)$$

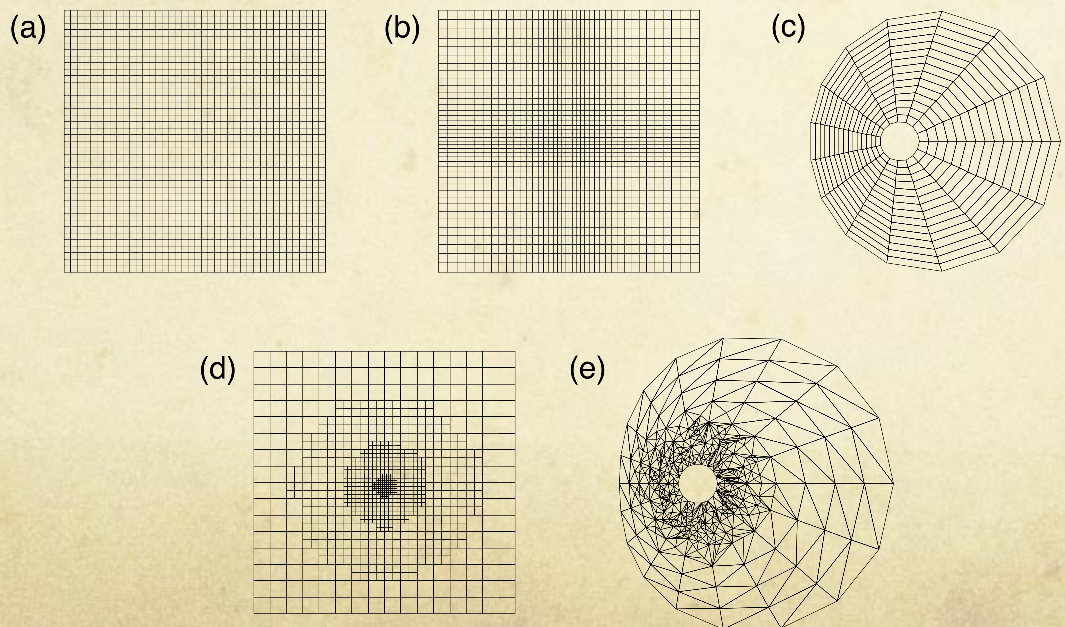
$$\boldsymbol{j} = \nabla \times \boldsymbol{B} \qquad (2g)$$

$$U = \frac{p}{\gamma - 1} + \frac{\rho v^2}{2} + \frac{B^2}{2} \qquad (2h)$$

Credit: *Raeder* (2003)

Numerical modeling

- In contrast to analytical solutions numerical modeling is done in discrete spatial and temporal domains.
- One thus needs to select a spatial simulation grid appropriate for the setting of interest. Common grids include:



a) uniform Cartesian, b) stretched Cartesian, c) spherical, d) adaptive Cartesian and e) unstructured grids (credit: *Raeder*, 2003)

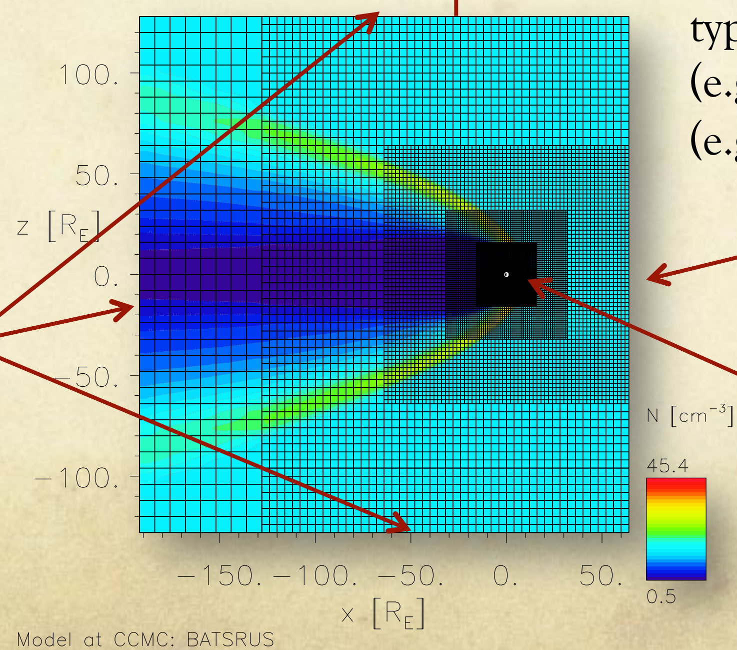
Numerical modeling

- Obtaining unique solutions to differential equations requires boundary and initial conditions.
- Typical boundary conditions in the global geospace simulations:

Typical BATS-R-US grid (credit: CCMC)

$\bar{n}$

$$\bar{n} \cdot \nabla \psi = 0$$



Dipole field used and plasma typically set initially to cold (e.g. 5000 K) and tenuous (e.g. 0.1 cm^{-3}) conditions

Solar wind (observations)

We will return to the inner boundary situation

Numerical simulations

- A great variety of numerical schemes developed to numerically integrate the equations of interest. Selection of appropriate scheme is a serious art.
- Integration generally divided into temporal and spatial components.
- Consider conservative form equation:

$$\frac{\partial U}{\partial t} = -\nabla \cdot \bar{F}(U) \tag{3}$$

Numerical modeling

- One common 2nd order (numerical truncation errors proportional to Δt^3) *time differencing* scheme reads:

$$
\begin{aligned}
U^{n+1/2} &= U^n - \frac{1}{2}\Delta t \nabla \cdot \bar{F}(U^n); \\
U^{n+1} &= U^n - \Delta t \nabla \cdot \bar{F}(U^{n+1/2})
\end{aligned}
\tag{4}
$$

This specific approach is called *explicit predictor-corrector scheme.*

Numerical modeling

- As a general rule of a thumb, smaller Δt (i.e. also more calculations) will give more accurate time differencing.

- For *explicit schemes* an important Courant-Friedrichs-Levy (CFL) stability criterion reads:

$$\Delta t_{\max} < \delta \frac{\min(\Delta x, \Delta y, \Delta z)}{|\bar{v}| + v_{MS}} \tag{5}$$

Of the order of 1

Flow and magnetosonic wave speeds

Tricks such as “Boris correction” limiting the wave speed can be applied. *Implicit schemes* can take larger time steps.

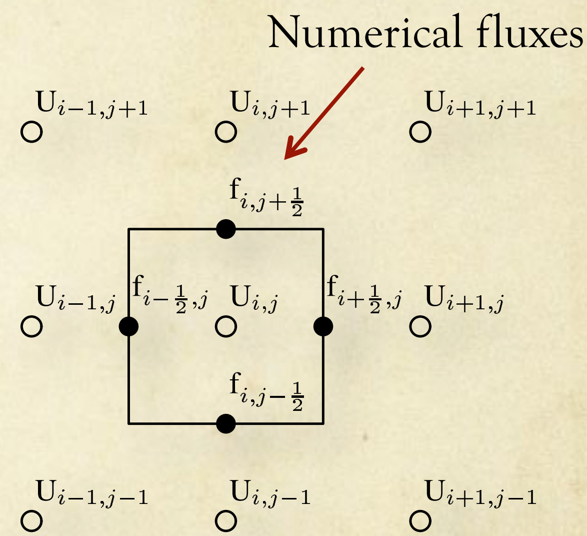
Numerical modeling

- Spatial differencing trickier. Again, many, many schemes available. Common *conservative finite differencing* scheme reads (see Eq. 3):

$$\frac{\partial U}{\partial t} = -\left(f_{i+1/2,j}(U) - f_{i-1/2,j}(U)\right)/\Delta x - \left(f_{i,j+1/2}(U) - f_{i,j-1/2}(U)\right)/\Delta y \qquad (6)$$

where 2nd order (numerical errors proportional to Δx^3) *central scheme* reads:

$$f_{i+1/2} = \frac{1}{2}\left(F(U_i) + F(U_{i+1})\right) \qquad (7)$$



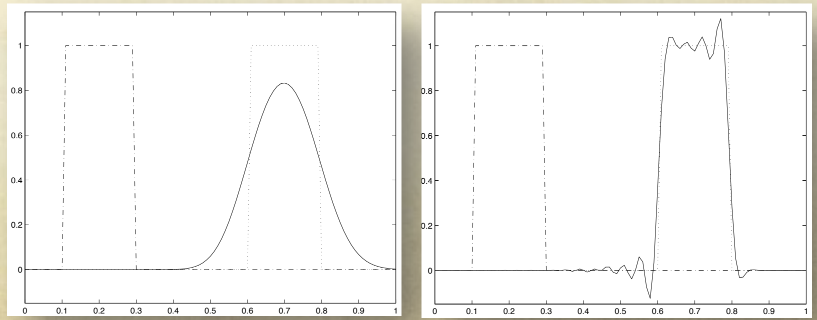
Cell centers and corners (credit: *Raeder*, 2003)

Numerical modeling

- The nature of numerical errors depends on the order of the spatial differencing scheme:
  - First order schemes (truncation error proportional to Δx^2) are *diffusive*. “Smoothing effect.”
  - Second order schemes (truncation error proportional to Δx^3) are *dispersive*. “Oscillation effect.”

- *Flux limiters*, for example, switching between diffusive and dispersive schemes used to find an optimal ground between the two effects.

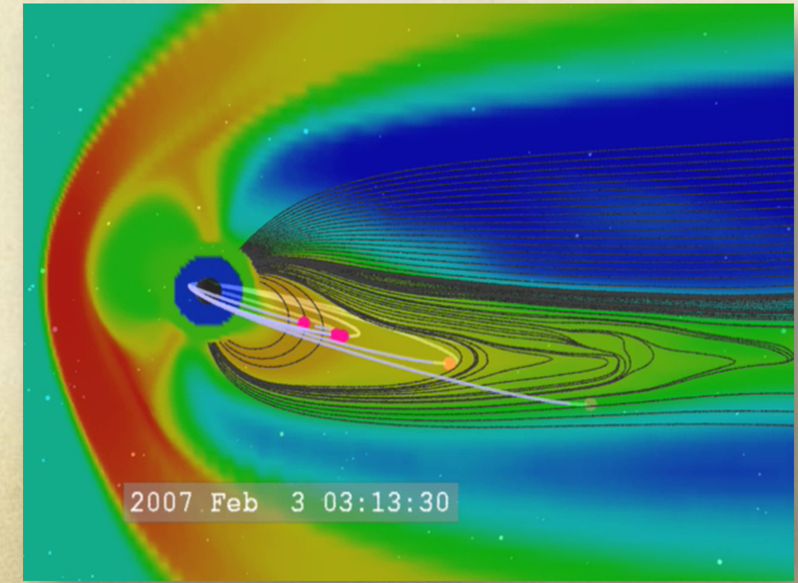
Examples of diffusive and dispersive solutions (credit: Prof. Kuzmin, U. of Erlangen-Nuremberg)



Numerical modeling

- Guaranteeing the condition $\nabla \cdot \bar{B} = 0$ in the numerical solution also requires some acrobatics but we will not go into those details here.

- So in the end, throw all the 4 ingredients into a bag, shake and something such as the following falls out:



OpenGGCM global MHD simulation of magnetospheric plasma density (credit: NASA GSFC SVS)

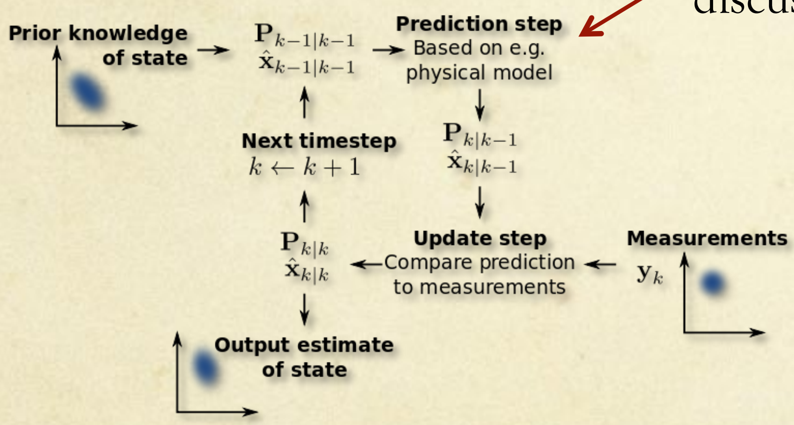
Numerical modeling

- No simulation is perfect and it is imperative to keep in mind some of the main potential sources for errors in the numerical modeling process:
  - Quality/accuracy of the physics captured by the equations that are being solved.
  - Quality of the boundary conditions – "garbage in garbage out."
  - Non-grid convergence – need more resolution.
  - Quality/accuracy of the used numerical schemes.

Numerical modeling

- Data assimilation that is widely used in regular weather predictions is becoming more common also in space weather applications:

Step we have been discussing past few slides



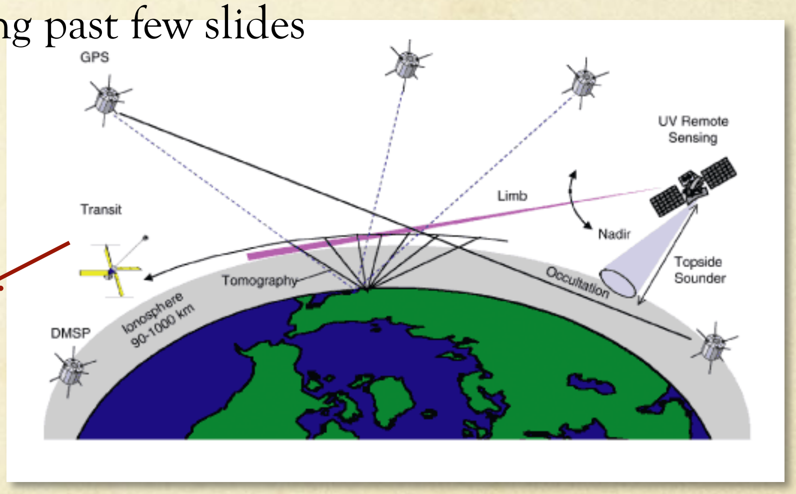
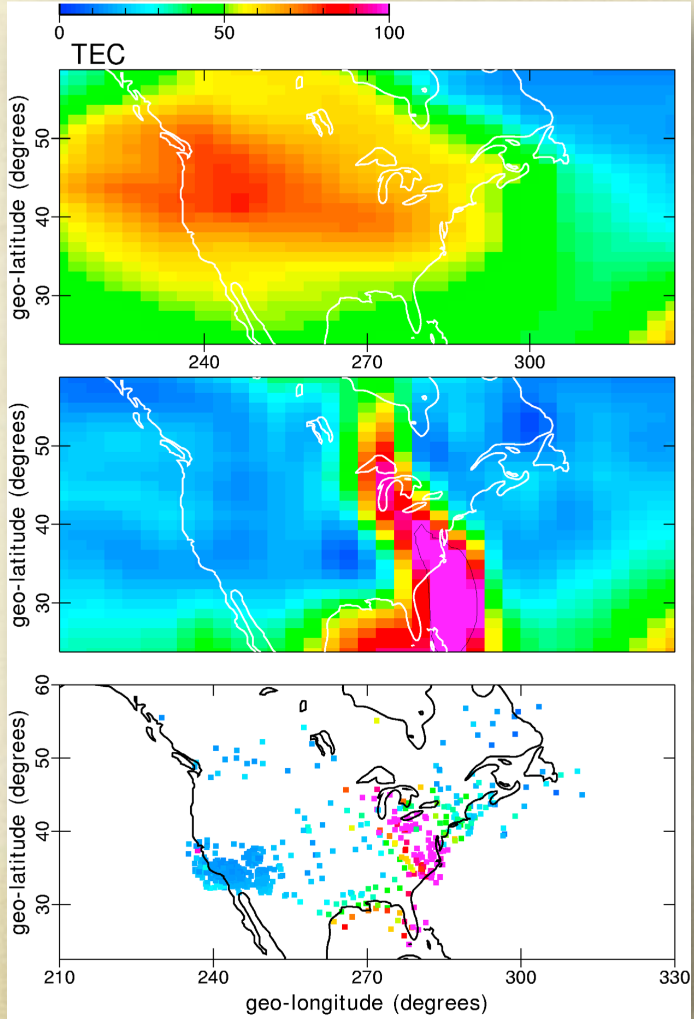


Illustration of the idea behind Kalman-based data assimilation (credit: Wikipedia)

Observations being ingested by GAIM (credit: Schunk et al., 2005)

Numerical modeling

- Data assimilation can provide substantial improvements to model predictions and is definitely one of the key areas for further future development.
- However, sparse nature of space weather data poses a challenge.



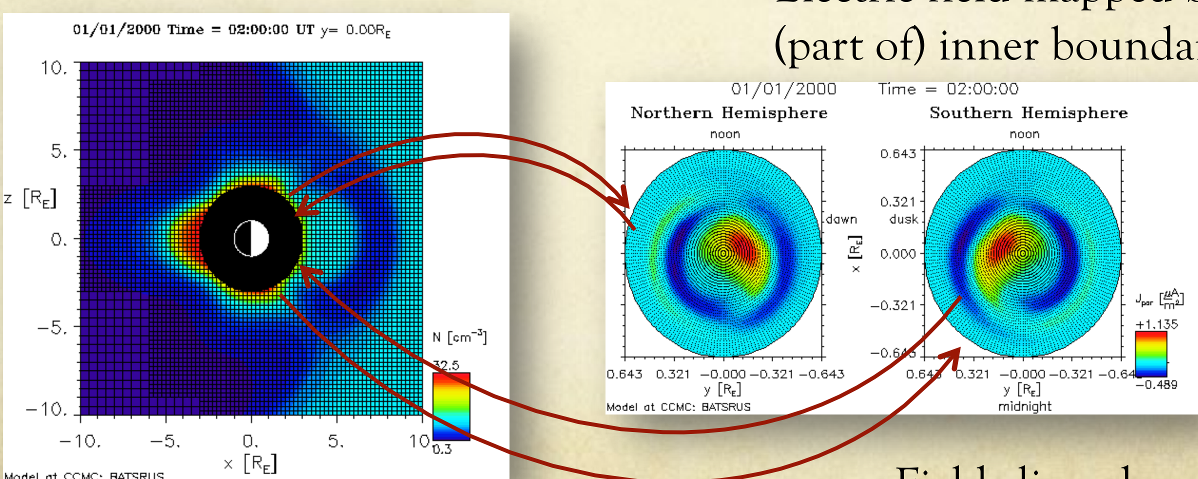
Top: GAIM forward model prediction without data assimilation, middle: GAIM prediction with observed TEC assimilated, bottom: TEC observations (credit: *Schunk*, 2012)

Numerical modeling

- A lot of recent progress in coupling different space weather models with each other: connecting different domains and different physics.

- Classic example is the coupling between global MHD and ionospheric electrodynamics:

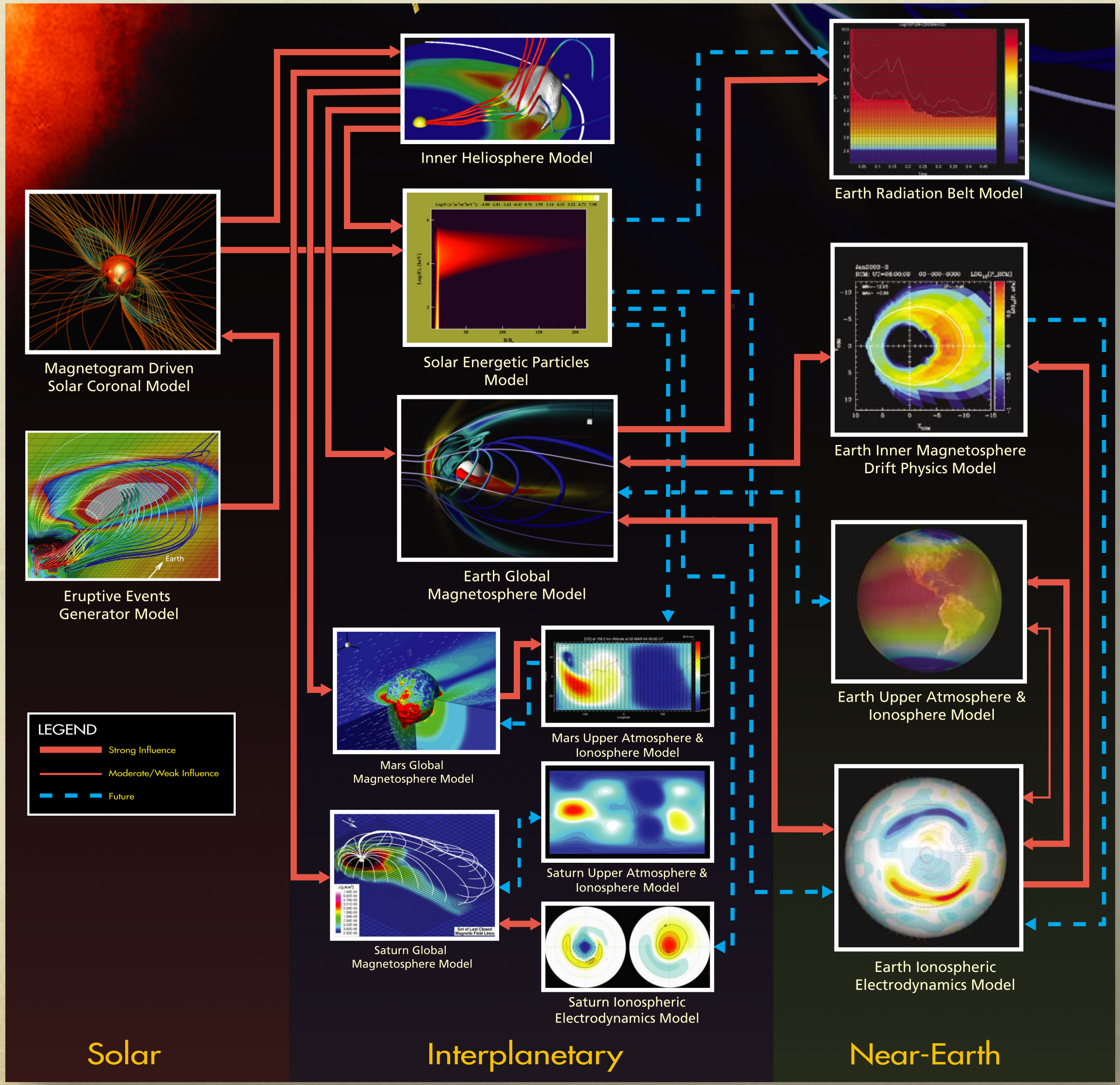
Electric field mapped back to provide (part of) inner boundary conditions



Field-aligned currents → solution for the electric field

Example global MHD and ionospheric domains (credit: CCMC)

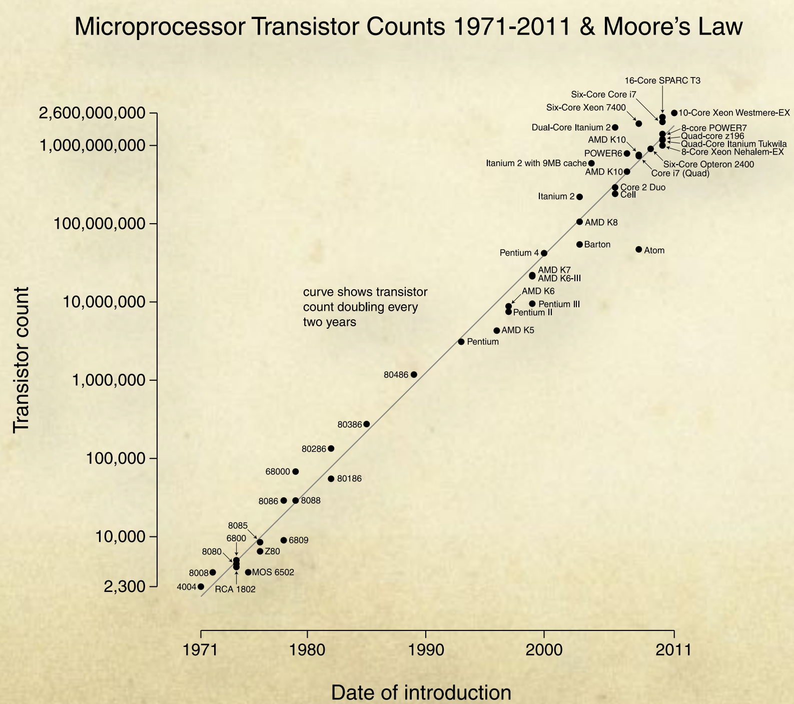
Numerical modeling



State-of-the-art: model coupling in the Space Weather Modeling Framework (credit: University of Michigan)

Numerical modeling

- Enhancement in the computational capacity has revolutionized also our capability to carry out numerical space weather simulations.

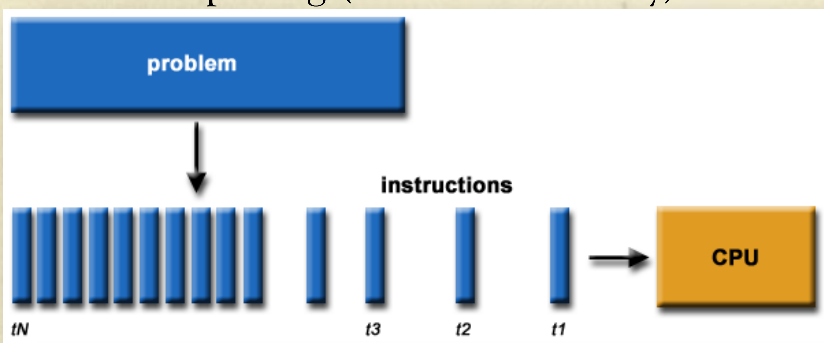


Number of transistors in integrated circuits and Moore's law (credit: Wikipedia)

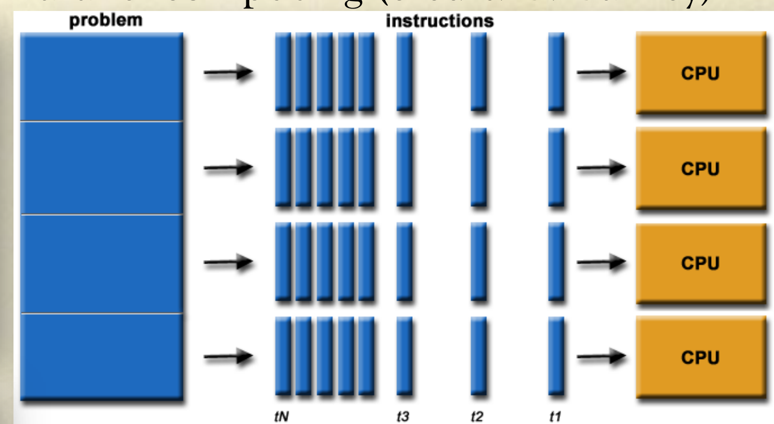
Numerical modeling

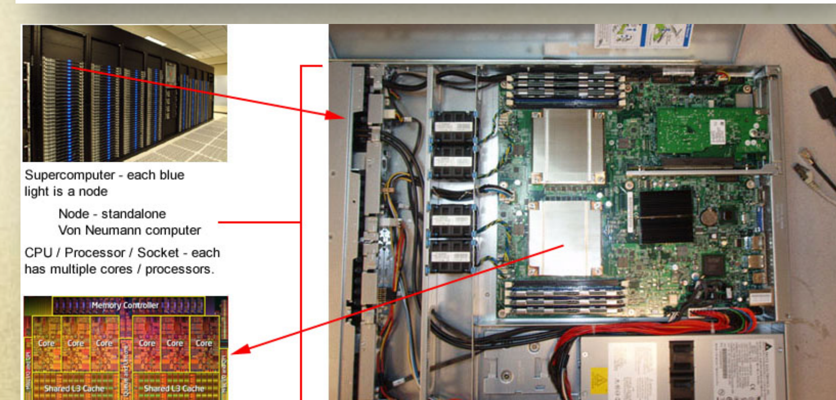
- However, there are limitations for making single processors even faster. The future is in *parallel computing*.

Serial computing (credit: B. Barney)



Parallel computing (credit: B. Barney)





Cluster supercomputer composed of nodes, CPUs and cores (credit: B. Barney)

Numerical modeling

- Running modern first-principles space weather models in real-time requires parallel code implementation and usage of, for example, Beowulf clusters.

Approx. 1000 CPU Beowulf system operated by CCMC and SWRC at NASA GSFC

15000 CPU "Discover" cluster at NASA Center for Climate Simulation (credit: NASA/Goddard/Pat Izzo)

Numerical modeling

- Let's then review briefly some of the latest first-principles space weather models.
- NASA GSFC Community Coordinated Modeling Center (CCMC) the largest single one-stop-shop for a good collection of these models.
- Many of these models are run in real-time and the results are available in iSWA.

Numerical modeling

- One should never blindly trust model predictions. One needs to understand how models performs in different situations.
- Model “error bars” can be studied through rigorous validation against observed physical parameters.
- CCMC has been leading community-wide model validation efforts for all major space weather domains.

Numerical simulations

- Let us then briefly review the basic steps for rigorous model validation. We will use recent validation of ground magnetic field predictions as an example.

- First ones needs to select the time periods of interest:

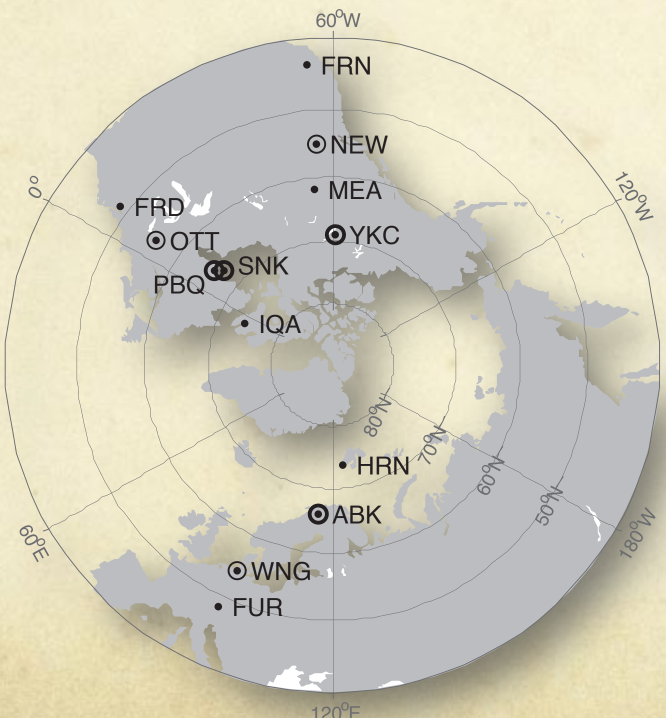
Table 1. Geospace events studied in the validation activity. The last two columns give the minimum Dst index and the maximum Kp index of the event, respectively.

Event #	Date and time	min(Dst)	max(Kp)
1	October 29, 2003 06:00 UT - October 30, 06:00 UT	-353 nT	9
2	December 14, 2006 12:00 UT - December 16, 00:00 UT	-139 nT	8
3	August 31, 2001 00:00 UT - September 1, 00:00 UT	-40 nT	4
4	August 31, 2005 10:00 UT - September 1, 12:00 UT	-131 nT	7
5	April 5, 2010 00:00 UT - April 6, 00:00 UT	-73 nT	7
6	August 5, 2011 09:00 UT - Aug 6, 09:00 UT	-113 nT	8

Storm events used in the validation effort (credit: *Pulkkinen et al.*, 2012)

Numerical simulations

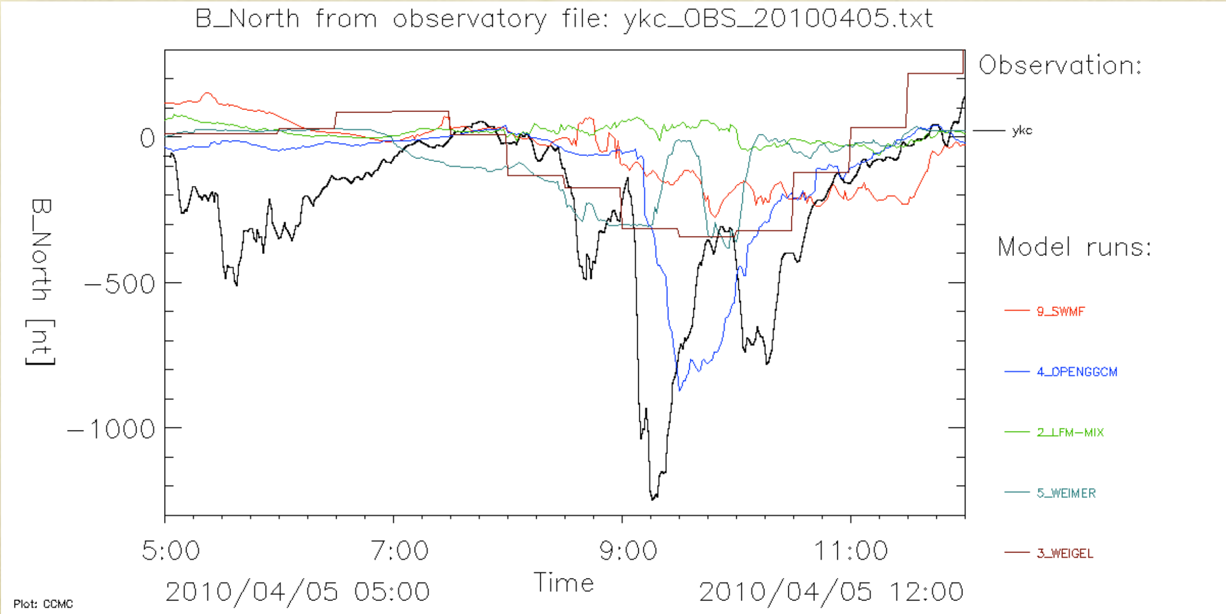
- Then one needs to find and select the sources for the observational data.



Location of the geomagnetic observatories used in the validation effort (credit: *Pulkkinen et al.*, 2012)

Numerical simulations

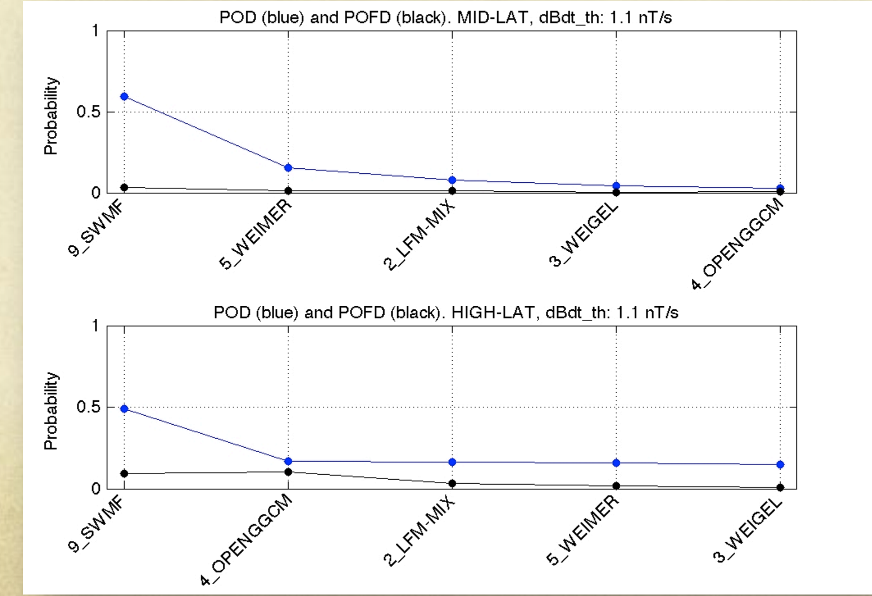
- Once the model(s) have have been run for the selected periods one can start comparing observed and predicted field variations.



Modeled versus predicted ground magnetic field variations (credit: *Pulkkinen et al.*, 2012)

Numerical simulations

- Finally one needs to quantify the model performance using some kind of *metric*. A zoo of different metrics available.
- We have recently used event-based metrics measuring models capability to detect threshold crossings within given time windows.



Probability of Detection (POD) and Probability of False Detection (POFD) within 20 min windows (credit: *Pulkkinen et al.*, 2012)

Tasks "Numerical modeling"

1. Request a global MHD simulation (do not use GUMICS because only serial implementation is available) at CCMC for the 4-5 hours of July 14, 2012 around the arrival of the CME at the Earth's orbit. Once the simulation has completed use CCMC's online visualization interface to study the modeled location of the magnetopause around the arrival of the CME. Submit your findings at https://docs.google.com/spreadsheet/viewform?formkey=dHN2X0RmcU1uNEdUdjVnQkM3eVo5VEE6MQ.

2. Watch tutorial http://www.youtube.com/watch?v=QAs73yvZ7eY on WSA-Enlil model and its use on space weather forecasting. Submit your findings at https://docs.google.com/forms/d/1vbfZVnGVpJnzjbm_283BqPO_81fotYl3Hwb5WY7jA6o/viewform.