Multiphysics Modeling
Simulating the Terrestrial Water Cycle

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Penn State University
Why HPC?
Issues & Opportunities

Multiphysics analysis is a unifying modeling strategy that allow scientists and engineers to explore fully-coupled effects of complex physical phenomena.

New sensors, communication networks, and characterization tools have made it possible to examine spatial and temporal phenomena over an unprecedented range of scales.

Environmental observatories are poised to take advantage of sensors and simulation tools to advance predictive understanding and environmental forecasting.

One measure of a new theory or formulation is its' ability to predict new phenomena. 3 examples.
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Architecture for Multiphysics Modeling

**Sequential Coupling Approach** one process or field is partially solved and then passed to the next physics field to form a partial solution. The iteration process continues until a final solution is achieved. The integration interface provides the services for subsystem interaction, data handling, mesh generation, parallel I/O, visualization, etc.

Mike Heath UIUC, 2008
Direct Coupling assembles all the physics equations in one matrix and solves all equations together. In this example an open-source GIS and Geodatabase is used for data management, mesh generation, space-time data analysis, and interface to the system solver and visualization.

Kumar, Bhatt, Duffy, 2008
Penn State Integrated Hydrologic Model: PIHM

Qu and Duffy 2007
## Semi-Discrete Approach

<table>
<thead>
<tr>
<th>Process</th>
<th>Governing equation/model</th>
<th>Original governing equations</th>
<th>Semi-discrete form</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel Flow</td>
<td>St. Venant Equation</td>
<td>( \frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} = q )</td>
<td>( \left( \frac{dc}{dt} = P_i - \sum Q_{ai} + \sum Q_{mi} + Q_{ai} - O_{ai} = E \right)_i )</td>
</tr>
<tr>
<td>Overland Flow</td>
<td></td>
<td>( \frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (vh)}{\partial y} = q )</td>
<td>( \left( \frac{dh}{dt} = P_o - I - E_o - O_o + \sum_{j=1}^{3} Q_{ij} \right)_i )</td>
</tr>
<tr>
<td>Unsaturated Flow</td>
<td>Richard Equation</td>
<td>( C(\psi) \frac{\partial \psi}{\partial t} = \nabla \cdot (K(\psi) \nabla (\psi + Z)) )</td>
<td>( \left( \frac{d \psi}{dt} = I - q^0 - ET \right)_i )</td>
</tr>
<tr>
<td>Groundwater Flow</td>
<td></td>
<td>( C(\psi) \frac{\partial \psi}{\partial t} = \nabla \cdot (K(\psi) \nabla (\psi + Z)) )</td>
<td>( \left( \frac{d \psi}{dt} = q^0 + \sum_{j=1}^{3} Q_{ij} - Q_i + Q_{gi} \right)_i )</td>
</tr>
<tr>
<td>Interception</td>
<td>Bucket Model</td>
<td>( \frac{dS_b}{dt} = P - E_i - P_o )</td>
<td>( \left( \frac{dS_b}{dt} = P - E_i - P_o \right)_i )</td>
</tr>
<tr>
<td>Snowmelt</td>
<td>Temperature Index Model</td>
<td>( \frac{dS_{snow}}{dt} = P - E_{snow} - \Delta w )</td>
<td>( \left( \frac{dS_{snow}}{dt} = P - E_{snow} - \Delta w \right)_i )</td>
</tr>
<tr>
<td>Evapotranspiration</td>
<td>Penman-Monteith Method</td>
<td>( ET_o = \frac{\Delta(R_n - G) + \rho_s C_p (e_e - e_s)}{r_s} \frac{r_s}{\Delta + \gamma (1 + r_s)} )</td>
<td>( \left( \frac{ET_o}{\Delta + \gamma (1 + r_s)} \right)_i )</td>
</tr>
</tbody>
</table>
Open Source Programming Tools

QGIS
- an open source and free "Programmable Geographic Information System"
- a mapping tool, a GIS modeling system, and a GIS application programming interface (API) all in one
- a platform independent Open Source Geographic Information System that runs on Linux, Unix, Mac OSX, and Windows
- libraries for raster and vector geospatial formats
- Object relational database is handled using PostgreSQL
- GRASS compatible

Qt/C++
- tools for programming the interface and visualization
<table>
<thead>
<tr>
<th>Feature/Time Series</th>
<th>Property</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>River</strong></td>
<td>Manning’s Roughness</td>
<td>Hernandez et. al., 2000</td>
</tr>
<tr>
<td></td>
<td>Topology: From Node – To Node, Neighboring Elements;</td>
<td>Derived using PIHMgis (Bhatt et. al., 2008)</td>
</tr>
<tr>
<td></td>
<td>Manning’s Roughness;</td>
<td>Dingman (2002)</td>
</tr>
<tr>
<td></td>
<td>Coefficient of Discharge</td>
<td>ModHms Manual (Panday and Huyakorn, 2004)</td>
</tr>
<tr>
<td></td>
<td>Shape and Dimensions;</td>
<td>Derived from regression using depth, width and discharge data from <a href="http://nwis.waterdata.usgs.gov/usa/nwis/measurements">http://nwis.waterdata.usgs.gov/usa/nwis/measurements</a></td>
</tr>
<tr>
<td><strong>Forcing</strong></td>
<td>Precipitation, Temperature</td>
<td>Gauge data obtained from MARFC. 6 hourly precipitation point data is spatially gridded such that it conforms to the monthly precipitation distribution map obtained from parameter-elevation regressions on independent slopes model (PRISM) (Daly et. al., 1994, 1997)</td>
</tr>
</tbody>
</table>
Conceptual Model + GeoDataBase = A Priori Data

Conceptual Model Groundwater flow in the Allegheny Plateau Section.

Example of the GIS for the surface geology coverage.
PIHM GIS Framework

User Interface

Data Management
- Vector Processing
- Raster Processing
- Data Model Loader
- Parameterization

PIHM
- Kernel Definition
- Numerical Solver

Data Analysis
- Spatial
- Temporal
- Spatio-Temporal
- Uncertainty

Field, Feature Objects, Non-Spatial Data

Data Access Tool
- (Grid-Shp/Dbf) Read
- (Grid-Shp/Dbf) Write

Geodatabase
(Schema, Data, Relationships)

Domain Decomposition
- Static: Conformed, constrained Delaunay & nested triangulation
- Dynamic: Adaptive triangulations
PIHM GIS Interface
Issues & Opportunities

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WSN Architecture

WWW PSU Backbone

UNIDATA Thredds Server

Base Station Gateway

5.2 GHZ Motorola Multipoint Network Range -10 km

WSN Mesh
2.4 GHZ
&
30m Tower
900 MHZ

sensors
WSN: Wireless Sensor Network

IRIS 2.4 GHz radio

Stargate Netbridge Gateway 7 Web Services

ASA

eKo
Soil moisture temp

MDA320 Sensor Board DAQ
Some Sensor Properties/Limitations

Heterogeneous sensors: observe the atmosphere, vegetation, surface and subsurface coherently

Development of data acquisition for heterogeneous sensors

Low power requirement limits availability of sensors

Tradeoff between cost, response time, sampling rate

Power/charging issues in forest canopies
# Sensors Node Design

<table>
<thead>
<tr>
<th>SYSTEM</th>
<th>ITEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Station</td>
<td>Netbridge Gateway</td>
</tr>
<tr>
<td></td>
<td>MIB520 Base Station</td>
</tr>
<tr>
<td></td>
<td>IRIS Wireless Sensor mote</td>
</tr>
<tr>
<td></td>
<td>MDA300</td>
</tr>
<tr>
<td>Node Type A</td>
<td>IRIS Wireless Sensor mote</td>
</tr>
<tr>
<td>Weather Station</td>
<td>MDA300</td>
</tr>
<tr>
<td></td>
<td>Davis # 7852 Rain Gauge</td>
</tr>
<tr>
<td></td>
<td>Aluminum, Tower and hardware</td>
</tr>
<tr>
<td></td>
<td>Davis #6450 Net solar radiation</td>
</tr>
<tr>
<td></td>
<td>Davis # 7911 anemometer</td>
</tr>
<tr>
<td></td>
<td>HTM2500 HUMIREL Temp-RH</td>
</tr>
<tr>
<td></td>
<td>41303-5A Gill 6 plate shield (Camp Sci)</td>
</tr>
<tr>
<td></td>
<td>Solar panel, charger and battery</td>
</tr>
<tr>
<td></td>
<td>Enclosure 8x4x5”</td>
</tr>
<tr>
<td></td>
<td>Alum tower + hardware</td>
</tr>
<tr>
<td>Node Type B</td>
<td>Decagon Soil Moisture</td>
</tr>
<tr>
<td>Subsurface</td>
<td>SensorTechnics PS9005GCS-SQ07893 pressure transducer</td>
</tr>
<tr>
<td></td>
<td>0-5 psig, 5m cable</td>
</tr>
<tr>
<td></td>
<td>Decagon Soil Matric Potential</td>
</tr>
<tr>
<td></td>
<td>IRIS Wireless Sensor mote</td>
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<tr>
<td></td>
<td>MDA300</td>
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<td></td>
<td>Enclosure 8x4x5”</td>
</tr>
<tr>
<td></td>
<td>Alum. tower and hardware</td>
</tr>
<tr>
<td>Node Type C</td>
<td>Decagon Leaf Wetness Sensor</td>
</tr>
<tr>
<td>Vegetation</td>
<td>Dynamax Sapflow Senor</td>
</tr>
<tr>
<td></td>
<td>PAR Sensor *</td>
</tr>
<tr>
<td></td>
<td>IRIS Wireless Sensor mote</td>
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<td>Enclosure 8x4x5”</td>
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<tr>
<td></td>
<td>Decagon Metric Potential</td>
</tr>
<tr>
<td></td>
<td>Enclosure</td>
</tr>
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</table>
Shale Hills CZO
Prototype Node

Web Services
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Integrated Modeling in a Coastal Watershed

Freshwater Discharge: Groundwater or Surface Water?

Smithsonian Environmental Research Center
Domain used in decomposition
Freshwater Discharge to the Chesapeake
Distributed Water Budgets
&
The Virtual Watershed

Mukesh Kumar, PhD 09
Little Juniata Watershed 875 sq km

Mukesh Kumar PhD 08
Distributed Stream Runoff in Upland
Spatial Mean ET from Distributed Simulation

b) Daily interception: $et_0 = 0.000584 \text{ m/d}$
c) Daily transpiration $et_1 = 0.000664 \text{ m/d}$
d) Daily ground ET: $et_2 = 0.000645 \text{ m/d}$
e) Monthly totals
f) Monthly percentages
Spatial Mean Energy & ET For Each Land Cover Type

(a) Daily Avg IS (m)
(b) Monthly Precip. (m)
(c) Monthly Tr (m/d)
(d) Monthly Rn (J/m^2/d)
(e) et0 (m/d)
(f) et1 (m/d)

Spatial Mean Energy & ET For Each Land Cover Type
Predicting Surface-Groundwater Interaction at Meanders Losing-Gaining Reach
Groundwater-Surface Water Interaction at Stream Junctions
Losing Stream
Predicting Gaining-Losing Stream Reaches
Predicted Distributed Stream Runoff at Outlet
Predicted ET-Groundwater Relation

Model transect

S4+S5 (m/d)

GW Depth (m)

Transect Distance (km)
A 2-D Finite Volume Model for Hydrodynamic and Sediment Transport in Rivers and Estuaries

Shuangcai Li
Department of Civil and Environmental Engineering
The Pennsylvania State University
PhD Dec 08
Hydrodynamic model: Shallow water equations

\[
\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (vh)}{\partial y} = 0
\]

\[
\frac{\partial (uh)}{\partial t} + \frac{\partial (u^2h + gh^2/2)}{\partial x} + \frac{\partial (uvh)}{\partial y} = -ghS_{ox} - ghS_{fx}
\]

\[
\frac{\partial (vh)}{\partial t} + \frac{\partial (uvh)}{\partial x} + \frac{\partial (v^2h + gh^2/2)}{\partial y} = -ghS_{oy} - ghS_{fy}
\]

Sediment transport model

\[
\frac{\partial (\phi h)}{\partial t} + \frac{\partial (\phi uh)}{\partial x} + \frac{\partial (\phi vh)}{\partial y} = E - D
\]

\[
\frac{\partial z}{\partial t} = \frac{D - E}{1 - p}
\]

Solute transport model

\[
\frac{\partial (\phi h)}{\partial t} + \frac{\partial (\phi uh)}{\partial x} + \frac{\partial (\phi vh)}{\partial y} = \nabla \cdot (K_h \nabla \cdot \phi)
\]
Malpasset Dam Break

- The Malpasset dam was located in Reyran river valley, about 12 km upstream of Frejus.
- It collapsed in Dec. 1959 due to the exceptionally heavy rain. There were 433 casualties.
- The simulation area is about 520 km$^2$
- The water level in the reservoir was 100 m.
- In the downstream of the dam, the bottom is set to dry since the discharge is unknown and small compared to the flood wave.
- The Manning coefficient is 0.033.
- The simulation is run to 2500 s on 26000 elements.
Motivation

Challenges:

Physical System

- Rapidly changing multi-scale flow (damaging) under extreme events;
- Interaction between hydrodynamics and transport;

Computational

- Complicated topography and geometry in real flow field;
- Wetting/drying processes, and very shallow flow;
- Stability, accuracy, and computational cost.
Topography of the Reyran valley and the coastal zone
Domain decomposition
Results

Flood inundation map

$t=0 \text{ s}$

$t=1000 \text{ s}$

$t=1500 \text{ s}$

$t=2000 \text{ s}$
Malpasset Dam Break Model & Observations

![Graph showing water surface level vs police survey points for different models and observations.](image-url)
Results

Flood inundation map

$t=2500$ s

$t=3000$ s
Computation & Observatory Science

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Multiphysics formulations will produce new predictions.

Open Source Code Sharing