Large-Scale High-Lundquist Number Reduced MHD Simulations of the Solar Corona using GPU Accelerated Machines

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We have recently carried out a computational campaign to investigate a model of coronal heating and current-sheet formation in three-dimensions using reduced magnetohydrodynamics (RMHD). Our code is built on a conventional scheme (pseudo-spectral, semi-implicit) and is parallelized using MPI. The current investigation requires very long time integrations using high Lundquist numbers, where the formation of very fine current layers challenge the resolutions achievable even on massively parallel machines. We present here results of a port to Nvidia CUDA (Compute Unified Device Architecture) for hardware acceleration using graphics processing units (GPUs). In addition to a brief discussion of our general strategy, we will report code performance on several machines that span a variety of hardware configurations and capabilities. These include a desktop workstation with commodity hardware, a dedicated research workstation equipped with four Nvidia C2050 GPUs, as well as several large-scale GPU accelerated distributed memory machines: Lincoln/NCSA, Dirac/NERSC, and Keeneland/NICS.

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Outline and Motivation

- Coronal Heating and the Parker Scenario, very brief introduction
- Reduced magnetohydrodynamics and our numerical scheme
- Describe our GPU/CUDA strategy and performance evaluation
- Future Directions & final comments
Coronal Heating Problem

- Corona (solar “atmosphere”): 1-2 MK
- Photosphere (solar “surface”): 5800 K
- Two key pieces of the puzzle:
  1) Random convection of photosphere
  2) Intense magnetic field protruding from photosphere into the Corona
- How does the magnetic field transmit and convert the kinetic energy of the photosphere and how does the coronal plasma and magnetic field respond?
- We investigate Parker's Model of “topological dissipation” (Parker 1972)
Coronal Heating: Topological Dissipation

- Parker coronal heating scenario (Parker 1972)

1. Sufficiently tangled fields cannot relax to smooth equilibrium
2. Current sheets form and heat the plasma ohmically while magnetic reconnection reduces topological complexity

TRACE 171 Å Fe IX/X \(\sim 1,000,000 \text{ K}\)
Coronal Heating: Scaling Simulations

- Goal of our study: Investigate how heating rate scales with dissipation coefficients as model evolves in statistical steady state

- Key challenges in computational study:
  1. Separation of scales required very high resolutions
  2. Need long time integrations for good statistics
Reduced Magnetohydrodynamics

- Magnetohydrodynamics (MHD):
  - Applies to electrically conducting fluids
  - Equations combine Navier-Stokes and Maxwell's Equations

- Reduced Magnetohydrodynamics (RMHD):
  - Low frequency limit of MHD, very well suited for simulations
  - Applicable in systems permeated by strong uniform magnetic field

\[
\begin{align*}
\frac{\partial \Omega}{\partial t} + [\phi, \Omega] &= \frac{\partial J}{\partial z} + [A, J] + \nu \nabla_\perp^2 \Omega \\
\frac{\partial A}{\partial t} + [\phi, A] &= \frac{\partial \phi}{\partial z} + \eta \nabla_\perp^2 A \\
B &= \hat{z} + B_\perp = \hat{z} + \nabla_\perp A \times \hat{z} \quad \text{--- magnetic field,}
\end{align*}
\]

\[\Omega = -\nabla_{\perp}^2 \phi \quad \text{--- vorticity,}\]

\[J = -\nabla_{\perp}^2 A \quad \text{--- current density,}\]

\[\eta \quad \text{--- resistivity,} \quad \nu \quad \text{--- viscosity,}\]

\[\phi \cdot A \equiv \phi_y A_x - \phi_x A_y\]

\[v = \nabla_{\perp} \phi \times \hat{z} \quad \text{--- fluid velocity,}\]
RMHD Numerical Scheme

- Adapted from Loncope (1993, 1994)
- Written in Fortran and MPI
- Predictor-Corrector time advance
- Finite difference, line-tied at ends in $z$
- Pseudo-spectral, Periodic in $x$-$y$
- MPI domain decomposition along $z$
• Formation of thin current layers.

\[ \eta = \nu = 0.00125 \]

(128x128x32)
• Formation of thin current layers.

\[ \eta = 0.0003125, \quad \nu = 0.000625 \]

(256x256x32)
Heating Rate Scaling

- Investigation is on-going, largest resolution so far is 512x512x64
Random drive in 3D RMHD

- Average energy dissipation rate saturated in small $\eta$.

Longcope & Sudan (1994):

$$\left\langle P_F \right\rangle \sim \nu_F \bar{B}_\perp \propto \eta^{-1/3}$$

$$\bar{B}_\perp \sim \left\{ l_F N_{eq}^{-1} \Delta^{-1/2} \right\}^{2/3} \eta^{-1/3}$$
Random drive in 3D RMHD

- Average magnetic field strength saturated in small $\eta$.

Note that $B_z = 1$.

Longcope & Sudan (1994):

$$\bar{B}_\perp \sim \left\{ l_p (N_{\tau_E})^{-1} \Delta^{-1/2} \right\}^{2/3} \eta^{-1/3}$$
Scaling analysis in 3D

Sweet-Parker reconnection:  \[ \frac{\delta}{\Delta} \sim S_\perp^{-1/2} \quad S_\perp \equiv \bar{B}_\perp w/\eta \]

Heating rate:  \[ \bar{W} \sim \eta N \Delta L \frac{B_\perp^2}{\delta} \sim \frac{\bar{B}_\perp^2 LL_\perp^2}{\tau_E} \]

If \( t_E < t_c \), no random walk:
\[ \bar{B}_\perp \sim B_z \frac{v_p \tau_E}{L} \sim \left[ \left( \frac{B_z v_p}{LN} \right)^2 \frac{L_\perp^4}{w\eta} \right]^{1/3} \]
\[ \bar{W} \sim \left( \frac{L_\perp^{10} B_z^5 v_p^5}{L^2 N^2 w\eta} \right)^{1/3} \]

If \( t_E > t_c \), random walk:
\[ \bar{B}_\perp \sim B_z \frac{v_p (\tau_c \tau_E)^{1/2}}{L} \sim \left[ \left( \frac{B_z v_p L_\perp}{L} \right)^4 \frac{\tau_c^2}{N^2 w\eta} \right]^{1/5} \]
\[ \bar{W} \sim \frac{L_\perp^2}{L} B_z^2 v_p^2 \tau_c \]

Substituting numerical parameters shows that transition at around \( \eta \sim 10^{-3} \)

RMHD Numerical Options for Improvement

- Largest resolutions we have used to date: 512x512x64 which requires months-long integrations
- Target resolutions: 1024 x 1024 x 128 and 2048 x 2048 x 256
- Pseudo-spectral portion of code dominates computation time
- Options for improvement: parallel FFT, CUDA, new algorithms
CUDA: CUFFT comparison with FFTW

- Benchark Nvidia C1060 +CUFFT vs. Intel Nehalem + FFTW
- Including transfer time, CUFFT only few times faster.
- Without transfer considered, the performance is phenomenal.
CUDA: Preliminary 2D port

- General strategy: maximize computational intensity:
  1. Do several FFTs per transfer
  2. Recycle memory of intermediate quantities
  3. Write simple kernels for point-wise arithmetic
CUDA: Tau Profiling – 3D port

- Profile now looks vastly different
- Extend to 3D preserving original MPI implementation
- Tau Profiling tool does not support CUDA but wrapping kernels is a practical workaround
Parallel Scaling Machine Summary

- Code benchmarked on several multi-gpu systems
- Tianhe 1A (current #1 on Top 500) included just for reference

<table>
<thead>
<tr>
<th>Name</th>
<th>System Type</th>
<th>SMP (Cores) (Speed)</th>
<th>Nodes (Mem)</th>
<th>GPUs</th>
<th>Node Interconnect</th>
<th>Pci-E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carver NERSC</td>
<td>IBM iDataPlex</td>
<td>Nehalem (8) (2.67 Ghz)</td>
<td>400 (24 GB)</td>
<td>None</td>
<td>Infiniband QDR</td>
<td>–</td>
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<tr>
<td>Lincoln NCSA</td>
<td>Dell Power-Edge 1950</td>
<td>Harpertown (4) (2.33 Ghz)</td>
<td>192 (16 GB)</td>
<td>96xS070 (GT200) 2 per node</td>
<td>Infiniband SDR</td>
<td>Gen 2 x8</td>
</tr>
<tr>
<td>Dirac NERSC</td>
<td>Testbed</td>
<td>Nehalem (8) (2.68 Ghz)</td>
<td>44 (24 GB)</td>
<td>44xC2050 (Fermi) 1 per node</td>
<td>Infiniband QDR</td>
<td>Gen 2 x16</td>
</tr>
<tr>
<td>Parker UAF Worksataion</td>
<td>Silicon Mech. Workstation</td>
<td>2xGulftown (12) (2.8 Ghz)</td>
<td>1 (48 GB)</td>
<td>4xC2050 (Fermi)</td>
<td>None</td>
<td>Gen 2 x16</td>
</tr>
<tr>
<td>Tianhe 1A NSCT (China)</td>
<td>NUDT TH-1A</td>
<td>Xeon (6) (2.53 Ghz)</td>
<td>7168 (36 GB)</td>
<td>M2050 Per node (Fermi)</td>
<td>NUDT Arch</td>
<td>Gen 2 x16</td>
</tr>
</tbody>
</table>
A GPU Workstation: Parker.gi.alaska.edu

- Four C2050 GPUs
- Two 6-core CPUs
- One GeForce GTX470 GPU
- Operating since Aug. 2010.
- ~$17,000
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UAF workstation (4 GPUs) can match performance of 32 Intel Nahelem chips (256 cores of Carver/NERSC)

- Overall performance boost is about an order of magnitude.
- Expect quasi-linear scalings to persist to larger node counts
GPGPU-New Machines

- An initial allocation has been granted for NICS/Keeneland
- Our NCSA/Lincoln allocation will be transferred to NCSA/Forge
- ORNL/Titan looks promising.

<table>
<thead>
<tr>
<th>Name</th>
<th>System Type</th>
<th>SMP (Cores) (Speed)</th>
<th>Nodes (Mem)</th>
<th>GPUs</th>
<th>Node Interconnect</th>
<th>Theoretical Peak Power</th>
</tr>
</thead>
<tbody>
<tr>
<td>Keeneland NICS/ORN (Phase 1)</td>
<td>HP SL-390 G7</td>
<td>Westmere (6) (2.93 Ghz)</td>
<td>120 (24 GB)</td>
<td>C2070 (6GB Fermi) 3 per node</td>
<td>Infiniband QDR</td>
<td>188 TF</td>
</tr>
<tr>
<td>Forge NCSA</td>
<td>Dell C6145</td>
<td>Magny-Cours (8) (2.33 Ghz)</td>
<td>36 (48 GB)</td>
<td>C2070 (6GB Fermi) 8 per node</td>
<td>Infiniband QDR</td>
<td>150 TF</td>
</tr>
<tr>
<td>Titan ORNL</td>
<td>Cray XE6</td>
<td>TBD</td>
<td>TBD</td>
<td>(Kepler?)</td>
<td>TBD</td>
<td>20 PF?</td>
</tr>
</tbody>
</table>
RMHD-CUDA Strong Scaling

Initial scaling results on Keeneland look very promising.
Summary & Future Work

- General strategy of maximizing computational intensity to exploit FFT performance on GPUs yields very positive result.
- Our RMHD CUDA code is in production on NCSA/Lincoln, NERSC/Dirac, NICS/Keeneland, and our UAF workstation.
- Overall we see about a 10X improvement over the previous best performance.
- There is room for improvement (exploit symmetry of real transforms, asynchronous transfers, concurrent kernels, fully employing CPU chip).
- Possible future work includes implementing four-field model.

References: