Experiences with the Dawn BG/P Platform for High Fidelity Semiconductor Device Simulations

LLNL Dawn User Forum (DUF)
User Presentation
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Sandia Pulse Reactor (SPR) testing provided qualification evidence in form of “Go/No-Go” decision.

SPR dismantled end of FY06.

Neutrons create damage.

Emitter (n-type)
Base (p-type)
Collector (n-type)

Damage degrades gain.

QASPR (Qualification Alternatives to Sandia Pulse Reactor) will provide a methodology to provide evidence for qualification via quantified uncertainty.

Slide courtesy of J. Castro.
RAMSES
Radiation Analysis, Modeling and Simulation for Electrical Systems

QASPR computational sequence

Neutron & gamma creation & propagation from reactor or nuclear burst
Neutron/Gamma Transport (NuGET)

Defect recoil-cascade formation
Neutron Collision/Damage Formation (Cascade)
(binary-collision approximation)

Defect & carrier reactions within recoil cascade
Defect Clustering (Cluster)

Finite-element device model with defect annealing
Device Performance (Charon)

Spice model
Circuit Model (Xyce)

Board & cable parasitics analysis

Slide courtesy J. Castro
Device Models Track the Transient Migration of Carriers and Defects Caused by Displacement Damage

Displacement damage degrades device gain.

Species & processes relevant for $T = 300$ K and times < 1 s.

- Si interstitial (I) (+2,+1,0,−1,−2)
- B$_i$ (+,0,−)
- B$_{iB}$ (+,0)
- C$_i$ (+,0,−)
- B$_{iO}$ (0,−)
- Vacancy (V) (+2,+1,0,−1,−2)
- VP (+,0,−)
- VO (0,−)
- VB (+,0)
- VV (+1,0,−1,−2)

33 species
~200 reactions

\[
\frac{\partial Y_i(x)}{\partial t} + \nabla \cdot J_i = R_i(x)
\]

\[
J_i = \mu_i E Y_i(x) - D_i \nabla Y_i(x)
\]

\[
-\nabla (\varepsilon \nabla \phi(x)) = -q(p(x) - n(x) + N_D^+(x) - N_A^-(x)) - \sum_{i=1}^{n} q_i Y_i(x)
\]

Slide courtesy of J. Castro
UQ process includes:
sensitivity analyses, calibration, and
uncertainty propagation

All these processes require ensembles of
calculations

UQ processes required at device and circuit
level (very iterative process)

Want to use highest fidelity models but
limited by computational viability

SA = Sensitivity Analysis
Computational Requirements for Semiconductor Device Simulations

- 2D bipolar junction transistor (BJT) with full defect physics $O(10^7 - 10^8)$ DOF; takes $O(\text{week})$ on $O(10^3)$ cores
- 3D simulations? $O(10^9 - 10^{10})$ unknowns
- Prediction plus uncertainly required for validation requires ensemble of calculations
  - 1D simulations presently (J. Castro et al.); $O(10^3)$ simulations
  - 2D could be performed on current largest platforms

1D
RAMSES/Charon Semiconductor Device Simulator

(Charon team: Hennigan, Hoekstra, Castro, Fixel, Pawlowski, Phipps, Musson, T. Smith, Shadid, Lin)

• Models the effects of radiation damage on semiconductor devices
• Drift-diffusion model; full defect physics for modeling damage to devices
• Massively parallel capability for high fidelity simulations
• FEM or FVM fully-implicit Newton-Krylov solver on unstructured meshes
• Fully-implicit Newton-Krylov robust; but need efficient solution of sparse linear systems
• SNL Trilinos solvers
  • Preconditioning
  • ML multigrid preconditioner
  • Currently using MPI-only portions of Trilinos
Preconditioners: Algebraic Multigrid for Semiconductor Problems
(w/ Shadid, Tuminaro, Hu, Siefert)

SNL Trilinos ML Library
(Tuminaro, Hu, Sala, Siefert, Tong, Gee)

- Algebraic multigrid has advantages over geometric multigrid for complex geometries
- Smoothed aggregation plus variant for nonsymmetric matrices

- Additive Schwarz domain decomposition preconditioners do not scale
- Need methods with global coupling such as multigrid

- Hypre (Falgout, Yang, Baker, Kolev, Tong, Chow, Lee, et al.) a very popular AMG library
Challenges of Debugging at Scale

- Algorithm that works well on 4k cores may not work well for 64k cores
- Alternative promising algorithm scales well up to ~4k cores, but what happens?
- How to debug at 64k cores?
- Print statements ?!?!?
- Need tools

- Steady drift-diffusion
Example Scalability Issue

Scaling of Comm_split for the case where the subcomm is the same as the communicator

<table>
<thead>
<tr>
<th>cores</th>
<th>Split time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8k</td>
<td>0.37</td>
</tr>
<tr>
<td>16k</td>
<td>1.6</td>
</tr>
<tr>
<td>32k</td>
<td>6.3</td>
</tr>
<tr>
<td>64k</td>
<td>28.2</td>
</tr>
<tr>
<td>128k</td>
<td>122</td>
</tr>
<tr>
<td>144k</td>
<td>154</td>
</tr>
</tbody>
</table>

- mpiP (Chambreau) indicated bottleneck was with Comm_split
Careful with MPI Implementation

Scaling of Comm_split for the case where the subcomm is the same as the communicator

<table>
<thead>
<tr>
<th>cores</th>
<th>bubble</th>
<th>quick</th>
</tr>
</thead>
<tbody>
<tr>
<td>8k</td>
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<td>0.11</td>
</tr>
<tr>
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<td>128k</td>
<td>122</td>
<td>0.29</td>
</tr>
<tr>
<td>144k</td>
<td>154</td>
<td>0.32</td>
</tr>
</tbody>
</table>

Message: Poor MPI implementation can hose a good algorithm

Message #2: When tracking down performance issues on $O(10^5)$ processes, tool are critical
Improvements While Working on BG/P

- Access to large number of cores critical to improving scalability
- BG/P: Reduced time by $7x$ for 2 billion DOF on 64k cores compared with first scaling study (Dec 2009)
- Bigger machines important, but algorithmic improvements still critical

- Steady drift-diffusion
Improved Scalability… But More Work to Do

• Time per iteration scales well
• But: preconditioner setup time, iteration count

• Close interaction with Trilinos team, so scaling improvements benefit other ASC codes
• Algorithms and scaling work directly benefited an SNL MHD project
• Hybrid MPI/threading/accelerators: Trilinos Kokkos and “next generation” templated software stack (also fixes 32-bit global int problem)
• Muelu: next gen ML (Hu, Gaidamour, Tumi etc.)

Scaled efficiency for time per iteration for 31,000 DOF/core (to 64k cores) and 10,000 DOF/core (to 147,000 cores)
Dawn BG/P Experience

- BG/P areas that could be improved
  - IBM C++ compiler buggy; poor templated code performance
  - Need alternative compiler, or GNU-built executable that worked
  - PowerPC slow, 1 GB RAM/core barely enough
  - Slow nodes (single bit errors); difficult when have 36k nodes
- BG/P has been a reliable platform
  - I/O always an issue for large machines, BG/P file system better than average
- BG/P an excellent resource to improve scaling
  - Platform has excellent scaling
  - Regular access to 64k cores (previously ~6k cores)
- Critical to have an unclassified porting/test platform
- Great support from LC
  - John G’s help to port code (and feed bugs back to IBM)
  - Others (e.g. Scott, Tom, Sheila, etc.)
Concluding Remarks and Future Work

- Algorithmic improvements critical for scalability and efficiency
- Access to large core counts on Dawn critical for improving scalability of algorithms
- Tools critical (e.g. mpiP)
- Algorithmic improvements impacted Charon Cielo acceptance testing work
- Other codes (including ASC codes) will benefit from algorithmic improvements
- Murphy’s Law exacerbated at scale: everything starts to break (app code, MPI implementation, tools, etc.)
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References:

