Application Performance Tuning Activities in LANL’s X Division

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What a LANL User Does

We want to look at something (V&V, Model parameter study, Design question, or the like), so we:

- Initial Setup
- Run Simulation(s) [CODES]
- Analyze Results
- Make Changes in Setup, Models, or Code
- Come to Conclusion

• Code *turnaround time* very important
• Memory use also key
  • Resolution
  • Compute Resources required
The Code Environment

• LANL Designers use a small number of codes in their work
  – F90, F77 (C/C++ used mostly as glue)
  – Tens to hundreds of PEs
  – Depending on study, a few to a few hundred separate calculations

• Codes contain a variety of algorithms and run on several platforms.
  – LANL work is mainly on ASC Q (Digital-Compaq-HP) and on Lightning (Linux cluster)…
  – …but other platforms are becoming interesting (Red Storm at SNL, Purple at LLNL)
“Problems” We Want to Help With

• Code Team work load
  – Can preclude performance work
  – Certainly precludes *systematic* performance work

• Communication
  – …*or lack thereof*, with outsiders
  – Latest tools may not filter in
    • Unaware of them
    • Learning curve
    • Filtering useful from not
The Current Team

• Core: 3 Staff members in Computational Methods group (X-8)
• I/O: 1 Staff member in HPC Systems Integration group (CCN-9)
• I/O & Tools: 2 Staff members in HPC Environments group (CCN-8)
FY 2006: Optimization “L2”

• “L2” milestone (6 FTE effort) on Weapons Code optimization
• Evaluate current performance
• Develop infrastructure to maintain performance data
• Design suggestions/implementations for better performance/efficiency
• Most important product: the team
Stakeholders

- ASC Program CS element funds 6 people: the “customer”
- ASC codes element – the code teams at LANL – provide some level of help and will benefit: the “clients”
- The Designers – users of the codes: the ultimate “clients”; they need to run more problems, and run them faster
We want to...

- Put the latest tools to work helping LANL codes
- Provide a base of expertise in efficient use of compute resources
- Serve the users of the codes by providing faster, more memory efficient codes
- Be a center of LANL code performance data
- Bridge the gap between CCS, CCN and X division efforts
Fast

• Performance characterization
  – Share data with relevant teams outside X-Div
    • CCS-3 PAL Team
    • CCN-8 Tools
    • CCN-9 File systems (partnership here for I/O optimization)
  – Interact with groups outside LANL
  – Close the loop – make recommendations

• Take Action
  – Plan and execute optimizations in the codes
  – Subject to teams’ testing and acceptance standards and SQA processes
Daily Life in the Code Optimization Team

• Cycle
  – Characterize/study
  – Plan modifications
  – Implement and test
  – Collect data on each step
    • Estimate vs. Actual {Time|Speedup|Similar}

• Work on the rhythm of the code teams
  – Follow their testing & acceptance processes
  – Tie work to release schedules
Some Current Activities

- Developed an instrumentation library in use in the main ASC codes at LANL
- Collected “typical” calculation setups for use in characterizations
- Extensive work examining I/O issues in the codes
- Initial characterizations
Transparency is Key

• Data on performance should be available
  – To the code team
  – To other LANL researchers

• Hiding it is no way to improve
  – Experts from outside team may be able to contribute
  – Performance problems - if they exist - don’t magically go away
  – The lab must fight against a culture where it would be used to punish teams or people
What We Can Do Together

- Tools in our team’s hands, and put at the disposal of the developers
- Process for using extra-LANL people and ideas
- Bring the latest computer science research to bear on the codes
- Increase outside interactions
Conclusions

• *Systematic* optimization
• An “engineering” orientation
• The important product: the team
• Building a center of expertise
  – In tool use
  – In characterization
  – In interactions within and without LANL
Thanks!
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