A look at trends in computational methods: the tie between machines and mission science

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40th Anniversary Lecture Series

LA-UR-21-23988
Discovery science happens in the intersection between machines & mission

- Broad trends in codes delivering “discovery science” for multiphysics applications
  - Machines
    - Nic Lewis gave a nice overview of platform development
  - Mission
    - Ray Juzaitis gave a nice overview of NNSA mission drivers throughout the ASCI and ASC eras
    - Examples from astrophysical transients
Pre-ASCI: Qualitative understanding from computation

1980’s

Architectures

- Vector

Code technologies

- 1D supernova simulations aimed at understanding energetics, timescales
- What is key physics in driving supernova explosions?

Mission/application drivers

- Blink comparison technology for finding supernova
- Experimental program is the glue
- Computation for trends

Detailed radiation hydrodynamic, and microphysics in 1D does not show robust explosions
## Pre-ASCI: Multi-dimension and multi-physics trends

### 1990’s

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<tr>
<th>Architectures</th>
<th>Code technologies</th>
<th>Mission/application drivers</th>
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<tr>
<td>• MPP</td>
<td>• More routine runs in multi-dimension</td>
<td>• Supernova 1987A</td>
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<td>• Supercomputer market crash</td>
<td>• Do we have the key physics yet?</td>
<td>• CTBT → Stockpile Stewardship</td>
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<td>• Reduction of Gov’t purchasing</td>
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<td>• Mod/Sim becomes the glue</td>
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<td>• Rise of the PC</td>
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**Thinking Machine CM-5**

**Herant et al. 1994**

**Shock radius vs time**

**supernova explodes**
ASCI/ASC: Quantitative; predictive capability

~mid-90s-2015

Architectures
- Commodity cluster parallel
  - Economic driver
  - Long-lived stability

Code technologies
- MPI standard
- New MPI parallel multiphysics codes
  - Zeus-MP; ASCI Flash, CHIMERA
- How much do the details matter?
  - Add more!

Mission/application drivers
- Automated detections
- Statistics of a population
- Multi-messenger astronomy

“Add more” mentality fit right in at the Labs!
ASC: Abstractions, modularity, open source
~2010 - now
Model form exploration, multi-scale models

Architectures
- Cluster parallel – diverse specialized hardware
  - GPU
  - *Component Tailoring*

Code technologies
- Community codes; frameworks
  - Athena++, Gizmo, AMReX
- Performance portability abstractions
  - Node level: e.g. Kokkos ...
  - System level: FleCSI ...
- Beyond Euler & continuum approximation
  - Brute force resolution is not an affordable path to improving our understanding
  - Code agility to facilitate novel methods exploration is a priority

Mission/application drivers
- Social media...on demand data
  - Machine Learning
  - Cell phones & wearable tech

- Stockpile modernization
  - PCF → SCDS; pivot in focus with new scope

Mission Capability Delivery Schedule
- Stewardship
- Capability
- Delivery

2010 - 2018

2009 IBM RoadRunner
2015 Cray Trinity
2018 IBM Sierra
Highlight 2 LANL efforts aimed at addressing challenge of machine diversity & evolving mission

Next generation platforms (NGP)

We and Livermore have advanced a strategy that explores two paths enabled by commercial trends

- Accelerated Architectures Enabled by Industry-Driven Architectural Trends Codedesigned to Application Demands
- Complex Simulation Architectures Leveraging Component-Level Customization Tailored for Application

NVIDIA partnership as a path to success

ATDM Next generation code (Ristra/NGC)

Design of a high level abstraction layer FleCSI to aid in efficient porting, and enable physics agility

- Abstraction layers Facilitate diverse implementations?
- Abstraction layers Automate the port?
- ATDM investment initial success in L1 milestone

Insulate from architectural diversity when possible

Codesign to optimize for our most complex workflows
NGC: Ristra design targets flexibility in a volatile future

Separation of concerns between physics expression and CS execution

**Ever changing scientific questions & Rapidly changing HPC hardware**
- Ristra is creating a *flexible and agile* toolkit for next-generation multi-physics
- FleCSI abstraction layer separates concerns of physics and CS developers
- Portage remap and link library connects meshes, packages, and codes

**Current codes are**
- Synchronous; Static; Difficult to extend

**Ristra codes aim to be**
- Asynchronous/Concurrent; Dynamic (compile- and run-time); Agile
- Open to new innovation in methods and CS

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**Traditional multi-physics code architecture**
- Limited Set of Question of Interest
- Application Domain Experts (Users)
- Traditional operator split
  - Multiplicative coupling
  - Synchronous

**Ristra multi-physics code architecture**
- Compile-time specialization
- Flexible and agile tool kit for next-generation multi-physics
- FleCSI abstraction layer separates concerns of physics and CS developers
- Portage remap and link library connects meshes, packages, and codes

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**Future mission**
- Future physics
- Future computers
FleCSI: High-level Design

FleCSI is a C++ programming system for developing multiphysics simulation codes

- Runtime Abstraction Layer & Interfaces
  - High-level user interface → application developers
  - Mid-level static specialization interface → computational scientists
  - Core data structures → computer scientists
  - Support for multiple backend implementations
    → MPI, Legion, HPX (distributed-memory)
    → Kokkos, Kitsune (shared-memory)

- Programming Model (task-based, data-centric)
  - Runtime, control, execution, and data models

- Topologies
  - Mesh topologies (structured & unstructured)
  - Tree topologies
  - Set topologies
ATDM investments have pointed a way to improve efficiency in deploying codes on emerging architectures

- FleCSI abstraction layer helps automate porting to new platforms

Each code ports to each architecture

FleCSI’s central model for data and execution can be ported once and all FleCSI-based codes benefit
Through the ATDM program, we developed a powerful capability to explore new multiphysics methods

- ATDM investments also facilitate algorithmic exploration, in addition to improving efficiency of porting to emerging platforms.

- disciplined and common development environment ease the integration of multiple physics package components.

- Demonstration of multi-scale methods (HOLO Transport; VPSC material strength).

- Recent ATDM L1 demonstrated this agility for new physics algorithm development and deployment.
NGP: Our plan for advances in platform technology build on a recent industrial capability for specialization

The world is adopting customization as the path to performance in the post-Moore era
- ARM is at the center of a broad industrial capability for tailoring

Japanese (MEXT) – Fugaku

Japan and Europe have shown great potential for HPC
- US Exascale effort bet on a single path with its $2B investment
A new LANL institutional investment helps position the US on a path for long-term gains in computing

- Based on new line of NVIDIA technologies
  - $80M, delivery in early FY23
  - First new family in 2 decades

- Broad spectrum of advanced technologies for laboratory applications
  - Multiphysics, Machine Learning, Analytics...
  - Platform for hardware studies

- Since it is an institutional system, we can dedicate time to partnerships
  - Universities, DOD and industry

We and NVIDIA have assigned leaders for a codesign partnership

- Libraries and Compilers
- Deep Learning
- Storage
- Networking
- Light House Applications
- Sparsity, Simulations
- Characteristics + Profiling
- Architectures
- Testbeds

A partnership with NVIDIA answers the hardest question: How do we influence much larger industry efforts?
Summary

- Current mission drivers and machines are once again forcing exciting innovation in the computational tools we use for discovery science.
- LANL’s recent ATDM efforts have laid the foundation for a code development environment that can meet those mission and machine drivers.
- Commercial trends are opening some great opportunities for transforming the nature of our computational toolkits
  - GPU machines are underwriting a boom in Machine Learning methodologies for a broad set of applications
  - ARM processors offer the opportunity for component tailoring efforts that is reinvigorating interest in deep codesign partnerships.