CUMULVS Tutorial

ACTS Toolkit Workshop

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Scientific Simulation Issues...

- Fundamental Parallel Programming
  → Synchronization, Coordination & Control
- Distributed Data Organization
  → Locality, Latency Hiding, Data Movement
- Long-Running Simulation Experiments
  → Monitoring, Fault Recovery
- Massive Amounts of Data / Information
  → Archival Storage, Visualization
- Too Much Computer, Not Enough Science!
  → Need Some Help...
Potential Benefits from Computer Science Infrastructure:

- **On-The-Fly Visualization**
  - Interactive Access to Intermediate Results
  - Attached as Needed, Minimize Overhead

- **Computational Steering**
  - Apply Visual Feedback to Alter Course / Restart
  - “Close Loop” on Experimentation Cycle

- **Fault Tolerance**
  - Automatic Fault Recovery / Load Balancing
  - Keep Long-Running Simulations Running Long
Collaborative Infrastructure for Interacting with Scientific Simulations:

- Run-Time Visualization by Multiple Viewers
  - Dynamic Attachment, Independent Views
- Coordinated Computational Steering
  - Model & Algorithm Parameters
- Heterogeneous Checkpointing / Fault Tolerance
  - Automatic Fault Recovery and Task Migration
- Coupled Models…
Collaborative Combustion Simulation

Collaborative Viewing and Steering Enables "What if?" Computational Science

- Telesteering
- Multiple Viewers
- Distributed Combustion Computation
- Utilizing Human and Physical Resources of Multiple DOE Laboratories
- Allows Remote Experts to View and Influence the Simulation
  - Drive simulation to interesting solutions
  - Close the loop on simulate-revise-simulate cycle
  - Enhance convergence of numerical algorithms
  - Avoid wasting computer resources on uninteresting or incorrect experiments
CUMULVS Visualization Features

⇒ Interactive Visualization
  * Simple API for Scientific Visualization
  * Use Your Favorite Visualization Tool

⇒ Minimize Overhead When No Viewers
  * One Message Probe, No Application Penalty

⇒ Send Only Viewed Data
  * Partial Array / Lower Resolution

⇒ Rect Mesh & Particle Data

⇒ Common (HPF) Data Distributions
  * BLOCK, CYCLIC, EXPLICIT, COLLAPSE

⇒ Soon Unstructured, Sparse & Adaptive Meshes…
Multiple Simultaneous Views

Density

Temperature
Multiple Distinct Views

C - spmd.f
  call stvfini[]
  call stvdecompdefine[]
  call stvfielddefine[]
  do
    call localWork[]
    call exchangeInfo[]
      
    call stvfsendtofe[]
  while !not done!

Instrument existing parallel code.

Cumulus attaches/detaches viewers from parallel simulation on-the-fly

Remote collaborators view different parts of simulation, simultaneously

Global View 1

Global View 2
CUMULVS Architecture
coordinate the consistent collection and dissemination of information to / from parallel tasks to multiple viewers

interact with distributed / parallel application or simulation
supports most target platforms (PVM / MPI, Unix / NT, etc.)
Instrumenting Programs for CUMULVS

- **CUMULVS Initialization ~ One Call (Each Task)**
  ⇒ Logical Application Name, # of Tasks
- **Data Fields (Visualization & Checkpointing)**
  ⇒ Local Allocation: Name, Type, Size, Offsets
  ⇒ Data Distribution: Dim, Decomp, PE Topology
- **Steering Parameters**
  ⇒ Logical Name, Data Type, Data Pointer
- **Periodic CUMULVS Handler**
  ⇒ Pass Control for Transparent Access / Processing
- **Typically 10s of Lines of Code…**
Local Allocation Organization

dataValues

dataDim=2

dataOffset[0]

Valid Data

dataSize[0]

dataSize[1]

dataAllocSize[0]

dataAllocSize[1]
CUMULVS Particle Handling

- Particle Data Fundamentally Different
  ⇒ Data Fields Encapsulated in a Particle Container
  ⇒ Explicit Coordinates Per Particle

- Particle-Based Decomposition API
  ⇒ User-Defined, Vectored Accessor Routines

- Viewing Particle Data
  ⇒ AVS Module Extensions
  ⇒ Tcl/Tk Slicer Particle Mode
CUMULVS
Steering Features

• Computational Steering
  ⇒ API for Interactive Application Control

• Modify Parameters While (Long) Running
  * Eliminate Wasteful Cycles of Ill-Posed Simulation
  * Drive Simulation to More Interesting Solutions
  * Enhance Convergence of Numerical Algorithms

• Allows “What If” Explorations
  * Closes Loop of Standard Simulation Cycle
  * Explore Non-Physical Effects…
Coordinated Steering

- Multiple, Remote Collaborators
- Simultaneously Steer Different Parameters
  - Physical Parameters of Simulation
  - Algorithmic Parameters ~ e.g. Convergence Rate
- Cooperate with Collaborators
  - Parameter Locking Prevent Conflicts
  - Vectored Parameters…
- Parallel / Distributed Simulations
  - Synchronize with Parallel Tasks
  - All Tasks Update Parameter in Unison
Parallel Model Coupling in CUMULVS

- Natural Extension to CUMULVS Viewer Scenario
  ⇒ Promote “Many-to-1” → “Many-to-Many”

- Translate Disparate Data Decompositions
  ⇒ Parallel Data Redistribution Among Shared Data Fields
    → `stv_couple_fields(fieldID, appname, fieldname, ... );`
  ⇒ Fundamental Model Coupling Capability
    → Next Step ~ Interpolation in Space & Time, Units Conversion...

E.g. Regional Climate Assessment

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CUMULVS Fault Tolerance Features

- Application Fault Tolerance
  ⇒ Automatic Detection and Recovery from Failures

- User Directed Checkpointing
  ⇒ User Decides What / Where to Checkpoint
  ⇒ Minimizes Amount of Stored Data

- Heterogeneous Task Migration
  ⇒ Restart Tasks on Heterogeneous Hosts
  ⇒ Restart is Automatically Repartitioned if Host Pool is of Different Size or Topology (Yikes!)

- Avoids Synchronizing Distributed Tasks
  ⇒ Asynchronous Checkpoint Collection and Fault Detection
  ⇒ Minimize Intrusion of Checkpoint / Restart
Run-Time Fault Monitor

- One Checkpointing Daemon (CPD) Per Host
  - Ckpt Collector / Provider
  - Run-Time Monitor
  - Console for Restart / Migrate
- CPDs Comprise Fault-Tolerant Application...
  - Handle Failure of Host / CPD
  - Coordinate Redundancy
  - Ring Topology
Rollback Versus Restart...

- Rollback Recovery:
  ⇒ Only Replace Failed Tasks, “Roll Back” the Rest
  ⇒ Elegant & Cool, But You Must…
  → Monitor ALL Communication for Restart Notification
  → Unroll Program Stack, Reset Comm & File Pointers…
  ⇒ Necessary for High Overhead Restart Cases

- Restart Recovery:
  ⇒ “Genocide” ~ Kill Everything & Restart All Tasks
  ⇒ Simple Approach, No Additional Instrumentation
  ⇒ Not as Efficient a Recovery in All Cases…
Checkpoint Data Collection

• Data from Each Local Task Collected/Committed
  → `stvCheckpoint();`

• Invoke When Parallel Data / State “Consistent”…
  ⇒ Highly Non-Trivial in General! (Chandy/Lamport)
  ⇒ Straightforward for Most Iterative Applications
    → Save Checkpoint at Beginning or End of Main Loop

• No Automatic Capturing of Other Internal State:
  ⇒ Open Files, I/O, Messages-in-Transit…
  ⇒ CUMULVS Assumes User Handles This Recovery
    → Can Be Done Manually Using Saved Checkpoint State
    → Future Extensions to Assist…
Manual Software Instrumentation

- SPDT 98 Case Study ~ SW Instrumentation Cost

<table>
<thead>
<tr>
<th>Instrumentation:</th>
<th>Seismic:</th>
<th>Wing Flow:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original Lines of Code</td>
<td>20,632</td>
<td>2,250</td>
</tr>
<tr>
<td>Vis / Steer System Init</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Vis / Steer Variable Decls</td>
<td>48</td>
<td>73</td>
</tr>
<tr>
<td>CP Restart Initialization</td>
<td>21</td>
<td>12</td>
</tr>
<tr>
<td>CP Rollback Handling</td>
<td>41</td>
<td>34</td>
</tr>
<tr>
<td>Total Instrumentation</td>
<td>204 ~ 1.0 %</td>
<td>188 ~ 7.7 %</td>
</tr>
</tbody>
</table>
### Checkpointing Efficiency

- **SPDT 98 Case Study ~ Execution Overhead**

<table>
<thead>
<tr>
<th>Experiment:</th>
<th>Seconds per Iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SGI:</td>
</tr>
<tr>
<td>Seismic - No Checkpointing</td>
<td>2.83</td>
</tr>
<tr>
<td>Seismic - Checkpoint for Restart</td>
<td>2.99</td>
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<tr>
<td>Seismic - Checkpoint for Rollback</td>
<td>3.03</td>
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<tr>
<td>Wing - No Checkpointing</td>
<td>0.69</td>
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<tr>
<td>Wing - Checkpoint for Restart</td>
<td>0.77</td>
</tr>
<tr>
<td>Wing - Checkpoint for Rollback</td>
<td>0.79</td>
</tr>
</tbody>
</table>

(Checkpointing Every 20 Iterations ~ every 15 sec to 4 mins…!)  

**Seismic Overhead:** 4-14% Restart, +1-3% Rollback.  
**Wing Overhead:** 8-15% Restart, +0-2.5% Rollback.
An Aside: PVM vs. MPI

- Comparison of Features and Philosophy
- Which One to Choose?
  ⇒ Both Useful for Given Application Needs…
- CUMULVS Issues
  ⇒ Internals and General Usage
PVM (Parallel Virtual Machine)

- Use Arbitrary Collection of Networked Computers as a Single, Large Parallel Computer
  ⇒ Workstations, PCs (Unix or NT) ~ Clusters
  ⇒ SMPs, MPPs
- Programming Model & Runtime System
  ⇒ Message-Passing ~ Point-to-Point, Context, Some Collective Operations, Message Handlers
  ⇒ Resource & Process Control, Message Mailbox, Dynamic Groups, Application Discovery
  ⇒ Fault Notification
Message Passing Interface Standard

- Library Specification for Message-Passing
  ⇒ Designed By Broad Committee of Vendors, Implementors and Users
  ⇒ High Performance on Massively Parallel Machines and Workstation Clusters
- Comprehensive Message-Passing System
  ⇒ Point-to-Point, Collective, One-Sided
  ⇒ Groups/Communicators, Topology, Profiling, I/O
  ⇒ Some Process Control (MPI-2 ~ MPI_SPAWN)
PVM vs. MPI: Different Goals

- **MPI**
  - Stable Standard, Portable Code
  - High Performance on Homogeneous Systems

- **PVM**
  - Research Tool, Robust, Interoperable
  - Good Performance on Heterogeneous Systems
PVM vs. MPI: Different Philosophies

• MPI
  ⇒ Static Model (~ MPI_SPAWN in MPI-2…)
  ⇒ “Rich” API (MPI-1 / 128, MPI-2 / 288)
  ⇒ Performance, Performance, Performance…

• PVM
  ⇒ Dynamic Model
  ⇒ “Simple” API (PVM 3.4 / 75)
  ⇒ Flexibility (& Performance)
Portability vs. Interoperability

• Portable:
  ⇒ Re-compile Source Without Modification on a Different System, with C, C++, Fortran Support
  ⇒ True of Both MPI and PVM.

• Interoperable:
  ⇒ Executables on Different Systems Communicate
  ⇒ PVM ~ Yes, MPI ~ Sometimes (Not Required)
  ⇒ Different MPI Implementations? IMPI ~ Soon…
  ⇒ Language Interoperability?
    → PVM ~ Yes, IMPI ~ Soon…
Performance vs. Flexibility

• To Be Flexible, You Must Pay the Price…

• Heterogeneity Overheads:
  ⇒ Data Conversion, Network Protocol Selection, Extra Message Headers (on top of Native Comm)…

• Choose the Lowest Common Denominator?
  ⇒ Not the Best on Any System.

• Performance Dictates Locally Optimal Solution.
  ⇒ Lose Interoperability…
Interesting Result

- You can build an MPI implementation that supports interoperability and system dynamics across different systems / languages (some already do ~ Mpich, LAM, IMPI…).

- But, given all these conditions:
  \[ \Rightarrow \text{It Would Perform About the Same as PVM}!! \]
Supporting MPI Applications in CUMULVS

- CUMULVS Works with MPI Applications! 😊
- But MPI Doesn’t Have Everything We Need (Internally)
  ⇒ Static Model, Minimal Operating Environment
  ⇒ No Name Service / Database, Fault Recovery / Notification?
  ⇒ MPI_SPAWN( )…? Proxy Server for Viewer Attachment?
- Existing CUMULVS Solution:
  ⇒ Applications Communicate Using MPI or PVM or ???
  ⇒ CUMULVS Viewers / CPDs Still Attach Using PVM
- Possible “Reduced-Functionality” MPI Version…?
  ⇒ Currently Under Development…
CCA "MxN" Parallel Data Redistribution

⇒ Builds on CUMULVS Viz & Coupling Protocols
⇒ CUMULVS & PAWS (LANL) Being Integrated

→ “MxN” Generalizes Capabilities of Both Systems
  * Point-to-Point versus Persistent Connections (a la Viz)
→ CUMULVS Complements PAWS Coupling Work
Future CUMULVS Plans (2 of 3)

CUMULVS as a Foundry to Forge New Technology

High-Performance Visualization
- **Full Parallel Integration** of Pipeline
- CCA “MxN” → “M x N x P x Q x R”!

Proposed “Fully Connected” User-Centric Simulation Cycle

Ornol

Scalable Visualization Cache Architecture

100s GBs
10s GBs
GBs
100s MBs

Data
Reduction & Filtering
Parallel Render

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Future CUMULVS Plans (3 of 3)

Feature Extensions…

• Application Interface:
  ⇒ Assist Manual Instrumentation of Applications
  → GUI, Pre-Compiler...

• Checkpointing Efficiency:
  ⇒ Tasks Write Data in Parallel / Parallel File System?
  ⇒ Redundancy Levels, Improve Scalability…

• Portability:
  ⇒ Other Messaging Substrates
  → Reduced Functionality / Direct Connect for CCA & MPI
CUMULVS Summary

• Interact with Scientific Simulations
  ⇒ Dynamically Attach Multiple Visualization Front-Ends
  ⇒ Steer Model & Algorithm Parameters On-The-Fly
  ⇒ Automatic Heterogeneous Fault Recovery & Migration

• Future Opportunities
  ⇒ Couple Disparate Simulation Models
  ⇒ Integrate as “MxN” Component in CCA
  ⇒ Application Instrumentation GUI / Pre-Compiler

http://www.csm.ornl.gov/cs/cumulvs.html
Seismic Example ~ 2D (Tcl/Tk)

Seismic Example ~ 3D (AVS)

Air Flow Over Wing Example ~ 3D (AVS)