Parallel PENTRAN Applications

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Overview

- Introduction
- Parallel Computing & MPI
- Boltzmann & Transport
- PENTRAN™ Code System
- Problem Solving Experience
- Discussion and Summary
- Questions
What is Parallel Computing?

- Computer with many processors
  - “Lumped” or *Network* “Distributed”
  - Divide problem up on processors

Serial...

- Task1
- Task2
- Task3
- RESULT

Parallel...

- Task1
- Task2
- Task3
- RESULT
About MPI...

MPI (Message Passing Interface) Library

- Began with “MPI Vendor Forum” May 1994
  - Formalized in 1995
- For distributed memory machines (FORTRAN, C, other language variants support)

ANSI-like “standard” in message passing

- Process com groups, parallel decomposition topologies
- Port code directly to architectures running MPI
- For any parallel architecture/cluster, SCANs
Amdahl’s Law: Limited Speedup

- (Parallel Code Fraction = $f$)
  
- $S_p = (1-f) + f/p + T_c/T_s$^{-1}
  
- Speedup = $S_p = T_s/T_p$, Efficiency = $E = S_p / P$
  
- If $f=0.8$, then max $S_p = 5.0$ as $P \to \infty$
Distributed Memory Programming

Efficient message passing algorithms...

- View message passing as a *last resort*
  - Minimize serialization, barriers
- Use a partitioned memory storage of data
  - Only way to solve *larger problems*
  - *Process mapping arrays* to determine “who’s where”

Overall...

- Use a coarse-grained code structure
- Many flops performed before messages passed
- Don’t forget about *Amdahl’s Law*
The 3-D Boltzmann Equation is given by:

\[
\begin{align*}
(\mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} + \xi \frac{\partial}{\partial z}) \psi_g(x, y, z, \mu, \varphi) + \sigma_g(x, y, z) \psi_g(x, y, z, \mu, \varphi) &= \\
\sum_{g'=1}^{G} \sum_{l=0}^{l} (2l + 1) \sigma_{l, g' \rightarrow g}(x, y, z) \{ P_l(\mu) \phi_{g', l}(x, y, z) + 2 \sum_{k=1}^{l} \frac{(l-k)!}{(l+k)!} P_k^l(\mu) \cdot \\
\left[ \phi_{C, g' \rightarrow g}(x, y, z) \cos(k\varphi) + \phi_{S, g' \rightarrow g}(x, y, z) \sin(k\varphi) \right] \} + \frac{x_g}{k_0} \sum_{g'=1}^{G} \nu \sigma_{g' \rightarrow g}(x, y, z) \phi_{g' \rightarrow g}(x, y, z)
\end{align*}
\]

- **Boltzmann Transport Equation**
  - Track particles traveling in different directions
  - over a range of energies
  - in different spatial locations in 3-D
Transport Theory

Boltzmann transport methods
- Monte Carlo method
- Discrete Ordinates (S_N) method
- Each has specific …

Advantages (+)

Disadvantages (-)

Issues

Both methods can take advantage of parallel processing!
Monte Carlo

Advantages

- Traditional, straight forward
- Geometrically precise
- Robust particle physics--Continuous-Energy xsec
- Parallelization obvious: particle histories

Disadvantages:

- Processing time, Non-analog variance reduction
- Inevitable uncertainties and Central LT
- “Global” solution difficult to obtain
- Results can be limited in application
Discrete Ordinates

Advantages

- Model entire geometry
- Fast and accurate
- Global flux distribution
- Directly allows for burnup, etc

Disadvantages:

- Proper multi-group cross sections
- Geometry discretized
- Memory, storage, differencing scheme issues
- Parallelization--coupling in angle, energy, space
Parallel Environment Neutral-particle TRANsporter

- Introduced in 1996, under continuous development that began in 1995 by Sjoden and Haghighat
- Parallel $S_N$ in $\text{angle}$, $\text{energy}$, and $\text{space}$ & $\text{I/O}$
- ANSI FORTRAN over 38,000 lines
- Industry standard FIDO input
- Solves 3-D Cartesian, multigroup, anisotropic transport problems
- Forward and adjoint mode, Fixed source, criticality eigenvalue problems
PENTRAN™

- Uses MPI Message Passing Interface library
  - Standard for MIMD systems
- Performs all I/O in parallel by each processor
- Uses a local, partitioned memory for memory intensive arrays (angular fluxes, etc)
- Auto-tuning feature for optimum memory allocation
- Builds processor communicators
  - minimized message traffic
  - communication across decomposition “planes” of processors
Performs automatic scheduling based on a user-specified decomposition weighting vector
Allows for adaptive differencing among coarse mesh zones using problem physics
Adaptive Differencing Strategy...
  - Diamond Zero (DZ)
  - Directional Theta-Weighted differencing (DTW)
  - Exponential-Directional Weighted (EDW)
  - Exponential-Directional Iterative (EDI) (see Feb07 NSE)
PENTRAN™

- Allows for a fully discontinuous variable meshing between coarse meshes
- Uses a novel higher order mesh coupling scheme: Taylor Projection Mesh Coupling (TPMC)
- Accelerations…
  - Two-grid 3-D TPMC-coupled “/” multi-grid transport acceleration
  - PCR with a zoned rebalance acceleration
- Multigroup & One-level SI schemes
PENTRAN™

- Allows for automatic Red-Black or Block-Jacobi
- Automatic load balancing
- Anisotropic scattering via Legendre Pn moments to arbitrary order
- 3-D angular quadratures level symmetric through S20, Legendre-Chebychev (Pn-Tn) to arbitrary order
- Vacuum, reflective, group-albedo boundaries
- Volumetric sources & plane surface fluxes
- PENDATA, PENMSH-XP utilities
PENTRAN

- Demonstrated 97% to 98% parallel fraction
  - Performance depends on problem, decomposition
  - Development focus on high accuracy & parallel efficiency
  - *Numerous applications over the past 12 years*

- Speedups of ~50 readily achievable
  - Demonstrated scalability
  - www.hswtech.com
Balance Equation...

\[
\frac{|\mu_m|}{\Delta x} (\psi_{\text{out}x} - \psi_{\text{in}x}) + \frac{|\eta_m|}{\Delta y} (\psi_{\text{out}y} - \psi_{\text{in}y}) + \frac{|\xi_m|}{\Delta z} (\psi_{\text{out}z} - \psi_{\text{in}z}) + \sigma \psi_A = q_A
\]

\[
\psi_{\text{out}x} = \frac{1}{\Delta y \Delta z} \int_0^{\Delta y} \int_0^{\Delta z} \psi_m(\Delta x, y, z) P_0(y) P_0(z) dy \, dz
\]
Taylor Projection Mesh Coupling

- Discontinuous grid densities
  - Allow high definition in ROIs, parallel load balance

First Order Taylor projection of angular fluxes at interface between discontinuous grid surfaces

- Flow Step
- Particle Balance Step
- Important for “Coarse to Fine”

\[
\psi_{inB} = \psi_{outA} + b A_y \frac{\partial \psi}{\partial y} \mid_A + c A_z \frac{\partial \psi}{\partial z} \mid_A + O(\Delta^2)
\]
A “Demo” Problem

- Annular region (38.1 cm OD) encompassing cylinder in x-y-z
  - k=1.00*, fast metal systems, 93.263% U-235 (tare U-238)
  - Placed in vacuum, non-metal regions are void

- 16-G Hansen-Roach MG xsecs
  - Zero pot dilute absorber O(MeV)n
  - <0.4% n groups 7 to 16 (< 17 keV)
  - Uncertainties lead to ~1%

*(KENO results from Wagner et al, 1992)*
Geometric Model Setup

- PENMESH-XP- automatically sets up problem
  - You define shapes, 3-D intervals, it does the rest...
- Example: Ring Problem, 4 coarse meshes:
Results: Ring Problem

GROUP 1

GROUP 2

GROUP 3

GROUP 4

GROUP 5

GROUP 6

$k = 0.994$

PENTRAN & MCNP-MG

10.109 cm thick

Cylinder Diameter, 17.78 cm

Annulus Inner Diameter, 27.94 cm
Venus-3 Shielding Problem

- Owned/operated by SCK-CEN in Mol, Belgium
- Practical model of a PWR
  - 16 "15x15" sub-assemblies, 1.26 cm pitch
- Types of fuel:
  - 4% enriched uranium, 3.3% enriched uranium
  - partial length 3.3% fuel upper/ stainless steel lower
- Other unique features
  - Water hole, SS baffle, Pyrex rods among 4% rods
- OECD Source, G1-26 of BUGLE-96, P3-S8
  - PENTRAN Runs for 4, 8, 16, 32 SP2 Processors
Venus-3 Shielding Problem

Figure 1a: Z-Level 1

Figure 1b: Z-Level 2

Figure 1c: Z-Level 3

Figure 1d: Z-Level 4
Venus-3

- PENMSH-XP code used to generate 3-D Cartesian Grid
- ~85,000 cells
- 26 Groups
- P3-S8 Discrete Ordinates

Group 1 Flux Solution:

Figure 2: 3-D Mesh and Material distribution of PENTRAN Venus-3 Model (upper reflector not shown)

Figure 3: Group 1 Flux Distribution for PENTRAN Venus-3 Model
Venus-3 Results

- Compared 370 Measured Rxn Rates (Ni, In, Al dosimeters) vs Integral Rxn Rates computed from PENTRAN P3-S8 26 group-dependent fluxes.
- 95% C/E values +/-10%; 5% within +/-15% (near P/L rods).
Comparison with others

C/E Equivalent Fission Flux for the $^{58}$Ni(n,p) reaction

<table>
<thead>
<tr>
<th>Detector Position Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>7</td>
</tr>
<tr>
<td>8</td>
</tr>
<tr>
<td>9</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>11</td>
</tr>
</tbody>
</table>

C/E Value

Comparison with others

- NEA (TORT)
- IKE-1 (TORT: r,theta,z)
- NRG (MCNP-4A)
- ORNL (DOT4+ANISN: Syn)
- KOPEC (TORT)
- IKE-2 (TORT: x,y,z)
- Spain (MCNP-4B)
- Siemens (TORT)
- PSU (PENTRAN)
- VTT (PREVIEW: DORT+Syn)
Comparison with others
C/E Equivalent Fission Flux for the $^{115}$In(n,n$'$) reaction

![Graph showing comparison of C/E values for various detectors and simulations]
Comparison with others
C/E Equivalent Fission Flux for the $^{27}$Al(n,$\alpha$) reaction

![Graph showing comparison of C/E values for various detectors.](image-url)
PENTRAN results are very close to experimental results; more than 95% of the Calculated-to-experimental (C/E) values are within ±10%, and only 5% of values within ±10% and ±15%.
### Table II: Dosimeter Number Locations in Regions of Venus-3

<table>
<thead>
<tr>
<th>Case</th>
<th>Processors</th>
<th>A/G/S Decomposition</th>
<th>Wall-clock Time, min</th>
<th>Speed-Up (4-node base)</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4 (1-set)</td>
<td>4/1/1</td>
<td>551.8</td>
<td>1.00</td>
<td>–</td>
</tr>
<tr>
<td>2</td>
<td>8 (2-sets)</td>
<td>8/1/1</td>
<td>311.9</td>
<td>1.77</td>
<td>88</td>
</tr>
<tr>
<td>3</td>
<td>16 (4-sets)</td>
<td>8/1/2</td>
<td>153.3</td>
<td>3.60</td>
<td>90</td>
</tr>
<tr>
<td>4</td>
<td>32 (8-sets)</td>
<td>8/1/4</td>
<td>84.3</td>
<td>6.54</td>
<td>82</td>
</tr>
</tbody>
</table>

HI-STORM Cask Simulation

- 24 PWR Assemblies
- 68 BWR Assemblies
- 1 Multi-purpose Canister (MPC)
- 6.7 cm for air flow gap
Spent Fuel Storage Cask Modeling

- Height ~ 610 cm
- Shell O.D. ~340 cm
- Shell I.D. ~187 cm
- Empty Weight 269,000 lbs (55.3 MT)
- Max. Loaded Weight 358,000 lbs (162.4 MT)
‘Large’ and ‘Small’ $S_N$ Cask Models

‘Large’ model has more meshes in the concrete and air.
Cask $S_N$ Models Summary

- **‘Large’ Model**
  - CASK library (22n, 18g)
  - 17 Materials
  - 318,426 fine meshes (1000 coarse meshes) (40 z-levels)
  - $P_3, S_{12}$ (168 directions)
  - 1.48 GB per processor
    8 processors (~12 GB Total)

- **‘Small’ Model**
  - CASK library (22n, 18g)
  - 17 Materials
  - 195,144 fine meshes (1000 coarse meshes) (40 z-levels)
  - $P_3, S_{12}$ (168 directions)
  - 1.15 GB per processor
    8 processors (~9.2 GB Total)
Cask 3-D Flux Distribution

Group 1

Group 22
Cask Comparison Four Annular Segments Near Source Centerline (300 cm), ‘Large’ Model

<table>
<thead>
<tr>
<th></th>
<th>Monte Carlo Results</th>
<th>PENTRAN/MC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A&lt;sup&gt;3&lt;/sup&gt;MCNP</td>
<td>MCNP</td>
</tr>
<tr>
<td></td>
<td>[(mRem/hr)/n/cm&lt;sup&gt;2&lt;/sup&gt;/s]</td>
<td>[(mRem/hr)/n/cm&lt;sup&gt;2&lt;/sup&gt;/s]</td>
</tr>
<tr>
<td>1.75E-04 (0.91%)</td>
<td>1.78E-04 (1.25%)</td>
<td>1.25E-04 (1.30%)</td>
</tr>
<tr>
<td>2.12E-04 (0.83%)</td>
<td>2.13E-04 (1.14%)</td>
<td>1.50E-04 (1.18%)</td>
</tr>
<tr>
<td>1.98E-04 (0.95%)</td>
<td>1.97E-04 (1.19%)</td>
<td>1.39E-04 (1.23%)</td>
</tr>
<tr>
<td>1.43E-04 (1.09%)</td>
<td>1.42E-04 (1.41%)</td>
<td>1.00E-04 (1.46%)</td>
</tr>
</tbody>
</table>

‘Small’ Model (PENTRAN/MC)
- Multigroup PENTRAN/MC average: 1.05
- Continuous PENTRAN/MC energy average: 0.74 (due to CASK MG library)
**Cask Model Timing Results**

MC is an average in four annular tally segments (Axial Mid-plane) 

(1σ Relative Error = 1%)

<table>
<thead>
<tr>
<th>Model</th>
<th># CPU</th>
<th>Dose Ratio to Reference</th>
<th>Run Time (hrs)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>A³MCNP Cont. Energy</td>
<td>1</td>
<td>1.00</td>
<td>109</td>
<td>1.5</td>
</tr>
<tr>
<td>Unbiased Cont. Energy</td>
<td>8</td>
<td>0.99</td>
<td>0.78</td>
<td>214</td>
</tr>
<tr>
<td>Unbiased Multigroup</td>
<td>8</td>
<td>0.70</td>
<td>0.46</td>
<td>362</td>
</tr>
<tr>
<td>PENTRAN ‘Large’ Model</td>
<td>8</td>
<td>0.74</td>
<td>165</td>
<td>1.3</td>
</tr>
<tr>
<td>PENTRAN ‘Small’ Model</td>
<td>8</td>
<td>0.74</td>
<td>123</td>
<td>1.7</td>
</tr>
</tbody>
</table>
## Cask Performance Comparison: $S_N$ and MC

<table>
<thead>
<tr>
<th>Model</th>
<th># CPU</th>
<th>Run Time (hrs)</th>
<th>Values/Hour</th>
</tr>
</thead>
<tbody>
<tr>
<td>A³MCNP Cont. Energy</td>
<td>1</td>
<td>2.5</td>
<td>1,856</td>
</tr>
<tr>
<td>Unbiased Cont. Energy</td>
<td>8</td>
<td>140</td>
<td>30</td>
</tr>
<tr>
<td>Unbiased Multigroup</td>
<td>8</td>
<td>220</td>
<td>19</td>
</tr>
<tr>
<td>PENTRAN ‘Large’ Model</td>
<td>8</td>
<td>165</td>
<td>42,100</td>
</tr>
<tr>
<td>PENTRAN ‘Small’ Model</td>
<td>8</td>
<td>123</td>
<td>35,000</td>
</tr>
</tbody>
</table>
BWR Core Shroud Problem

- BWR reactor and Core Shroud Assembly...
- ...with baffles, jet pumps, steam voids, etc.
- (Top) 67 Group P3-S8 coupled neutron-gamma calculation
- 265,264 fine mesh cells
- Solved in 12 hours on 48 IBM-SP2 processors, 8 processors angular, 6 processors spatial decomposition.
Displacement per Atom (DPA) in the core shroud shows intense radiation damage where fuel is close to the shroud.

Results were verified independently by Monte Carlo computations.

Multigroup PENTRAN (using BUGLE-96) values were within 5-15% of continuous energy MCNP values.

(Kucukboyaci, et. al, 2000).
C5G7 MOX Benchmark

- OECD/NEA C5G7 MOX 2-D Benchmark Problem
- PENTRAN Mesh distribution
- Specific pins represented among 229,551 spatial meshes
- S16 quadrature (228 directions)
- 7 groups
C5G7 MOX Benchmark Results

- **PENTRAN power distribution**
  - $k_{eff}=1.18760$
  - within <0.1% of MCNP
- **Relative power difference from MCNP**
  - avg difference is 0.88%
  - Compared to a statistical MC error 0.4% to 1.24%.

- **3-D unrodded case**
  - modeled with 946,080 spatial mesh cells
  - $k_{eff}=1.14323, +/-<0.09\%$ of MCNP
  - (Yi and Haghighat, 2004).
Recent Work for Industry

- Gamma transport problem/assessment

0.5 MeV forward

0.5 MeV adjoint

relative to detector response

0.15 MeV forward

0.15 MeV adjoint
Recent Work for Industry (2)

Relative Dose as a Function of Source Height

- Gamma transport problem/assessment
PENBURN 3-D Burnup Module

- Sponsored by the US Air Force
- Goal: Construct a 3-D zoned fuel burnup solver compatible with multiprocessing
- Solution of nuclide chains is obtained via quasi-static burnup steps
  - Explicit Bateman solver
- Distribute chains across processors

![Diagram showing the interaction between GMIX, PENTRAN, and PENBURN modules.](image)
PENBURN 3-D Burnup Module (2)

Bateman’s equations are stored using “path matrices” with “chain-linking precursors”

\[
N_i = \sum_{l=1}^{i-1} \left[ N_0 \xi_1 \xi_{i+1} \cdots \xi_{i-l} \left( \sum_{k=1}^{l} \prod_{\kappa \neq j} (\mu_k - \mu_j) \right) \right] + N_0 e^{-\mu t}
\]
X-Ray Modeling ...

- 90 m³ room discretized into ~131,000 3-D cells
- PENMSH™ code (8 “z-levels” floor to ceiling)
- BUGLE-96: last 4-group photon xsecs
- 80kV radiographic W-anode 32 mAs x-ray burst
  - Rotating anode water cooled source
- Hybrid X-ray Spectrum
  - Characteristic X-rays
  - Bremsstrahlung continuum
X-Ray Modeling ... “z-level 3”

Figure 2. z-level 3: 86.6 cm to 100.44 cm along z-axis.
X-Ray Dose, z=100 cm
Conclusions

- Parallel Computing
  - Deterministic Transport: PENTRAN™ Code System
  - Wide Variety of Problems
  - Automatic Mesh generation, adaptive numerical differencing, grid projections
  - Acceleration schemes

- In 2007, emphasis on Whole Core 3-D Transport Modeling

- Questions?