Continuous Energy Neutron Transport

Kevin Clarno

Mark Williams, Mark DeHart, and Zhaopeng Zhong

A&M Labfest - Workshop IV on Parallel Transport
May 10-11, 2005
College Station, TX

clarnokt@ornl.gov
(865) 241-1894
We need continuous energy transport when simple weighting functions fail.

\[ \sigma_g(r) = \frac{\langle \sigma(r,E) W(r,E) \rangle_g}{\langle W(r,E) \rangle_g} \]

- \( \sigma(r,E) \) = energy dependent XS from ENDF/B
- \( W(r,E) \) = weight-function that approximates neutron energy spectrum in system
- \( \langle \rangle_g \) means integration over the energy range in group ‘g’

You must know the solution to get the right cross section.
Variation of $^{238}\text{U}$ XS with energy
Variation of $^{238}$U XS with energy (100 – 1000 eV)
Problem-Independent XS

- Infinitely-moderated flux spectrum
  \[ W(r, E) = \phi_{\infty}(E) \]
  \[ \phi_{\infty}(E) = \begin{cases} \chi(E) & E \in \text{high energy range} \\ \frac{1}{E} & E \in \text{resonance range} \\ Maxwellian & E \in \text{thermal range} \end{cases} \]

- Self-Shielding
  - Simple improvements account for the effect of an isotope’s resonance on the spectrum that is used to weight it’s own MG cross section
Resonance cross section of $^{238}\text{U}$ using $\phi_\infty(^{238}\text{U})$ weight function.

\[ \sigma (\text{barns}) \]

\[ (E-E_0)/(\Gamma/2) \]

Flux

Group Cross-section

Cross-section
Resonance XS of $^{238}\text{U}$ using spectrum of 0.1\% $^{238}\text{U}$ diluted in H is 200x larger
Spatial dependence of XS is significant.

U-238 Capture XS: 30-100 eV

Flux Spectrum (1-3 keV detail)
CENTRM and GEMINEUTRON

- **What:** Solve 1-D/2-D DO transport to obtain a space-dependent, near-continuous-energy spectrum
- **Why:** To determine a problem-specific weight function to calculate the multi-group cross sections for other codes/applications.
- **How:**
  - PW data is pre-processed directly from ENDF/B data files (up to $10^6$ points per isotope)
  - Problem-specific energy mesh is determined
  - When weight functions are accurate, multi-group transport is used
    - Upper energy range where there are no resonances, and thermal range as an option
    - Temperature variation can be included within each material
    - Computes the anisotropic scatter source for each point “analytically”
Calculation of the scatter source is the key.

- 3/4-D phase space for each of ~30,000 points
  - Group-squared scatter matrix is huge and expensive
  - How can we get around this?
- Assume scattering is isotropic in the COM frame
  - Leads to anisotropic scatter in the lab system
  - “sub-moment” method separates $E' \rightarrow E$ terms into a product of $H(E)$ and $H'(E')$
  - ‘sub-moments’ lead to efficient evaluation of scatter source
- Includes PW thermal spectrum calculation with $S(\alpha,\beta)$ scattering
Efficient methods / acceleration

- Source-driven problem – no outer iterations
- Nearly purely-absorbing for each point
  - Almost any interaction changes the energy of the neutron
  - Very few inner iterations are required
  - In 1-D, even with reflecting boundaries, emission and absorption are easily computed analytically after a single transport sweep for each ordinate.
  - In 2-D, a similar Boundary Projection method is used.
- MG thermal-scattering is accelerated with multi-grid diffusion
Parallelization is necessary for improvements.

- 30,000 source-driven 1/2–D neutron transport calculations
  - Transport sweeping is 20-80% of total run-time
  - Source derivation is 20-80%
  - Many fuel pins are modeled – 1-4 min/pin

- Parallelization is in progress:
  - Directed towards few-processor systems
  - Spatial/Nuclide DD for the source
  - Angular DD for the solution
    - Spatial will be implemented in the future
Computational Performance for GE12 ESBWR Full Assembly

S4, P1 Calculation is performed

Energy Structure:
Total # of Energy Points in PW range: 32604

Geometry:
Total # of cells: 4318
Total # of external surfaces: 96

Material:
Fresh Fuel: UO₂ and Gd Rod
# Performance on CPILE Linux Cluster

<table>
<thead>
<tr>
<th>Number of Processors</th>
<th>Transport Sweep</th>
<th>2) Scattering Source</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1\textsuperscript{)T}_{\text{Com}} (min)</td>
<td>Total (min)</td>
<td>Speed up</td>
</tr>
<tr>
<td>1</td>
<td>636</td>
<td>54</td>
<td>690</td>
</tr>
<tr>
<td>2</td>
<td>314</td>
<td>30</td>
<td>344</td>
</tr>
<tr>
<td>3</td>
<td>218</td>
<td>23</td>
<td>240</td>
</tr>
<tr>
<td>4</td>
<td>163</td>
<td>16</td>
<td>180</td>
</tr>
<tr>
<td>6</td>
<td>122</td>
<td>15</td>
<td>136</td>
</tr>
<tr>
<td>12</td>
<td>76</td>
<td>12</td>
<td>88</td>
</tr>
</tbody>
</table>

1\textsuperscript{)} Communication Time, Minutes
2\textsuperscript{)} Scattering Source Calculation
Conclusions and Future Work

- Better solutions:
  - $k_{\text{inf}}$ is 2-5x better than self-shielding (< 2 mk)
- Potential for more local investigations:
  - Spatial flux distribution in compacts with particle fuels
  - Space and temperature effects on fuel performance
- Parallel performance:
  - This is just the beginning – Teresa will make it all fly!
- 3-D neutron/gamma transport
  - Full-core, time-dependent, point-wise eigenvalue calculations?
  - $10^9$ tets, $10^5$ points, $10^2$ angle, $10^x$ time steps
  - Petabytes and Petaflops
  - Necessitates multi-grid acceleration in $r$, $E$, and $\Omega$