Title: MCNP5 WORKSHOP - PHYSOR-2004

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Los Alamos
NATIONAL LABORATORY

mcnp
**Diagnostics
Applications
Group (X-5)**

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NATIONAL LABORATORY

MCNP5 Workshop

Forrest B. Brown & Russell D. Mosteller

Monte Carlo Development Team

Diagnostics Applications Group (X-5)
Los Alamos National Laboratory
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MCNP5 is a general-purpose Monte Carlo code used for neutron, photon, electron, or coupled neutron/photon/electron transport. The code has general 3D geometry modeling capabilities and uses detailed pointwise cross-section data for all physics interactions. Continued support for MCNP provides opportunities for the development of advanced Monte Carlo methods in many areas. This workshop will provide information on improvements and enhancements to MCNP5 which are of special interest to reactor physicists, including:

– New features in the MCNP5 code

– Parallel calculations on Linux clusters and ASC teraflop systems

– New nuclear data libraries for MCNP5

– Stationarity detection and dominance ratio for eigenvalue calculations

– Automated variance reduction for MCNP with deterministic adjoint calculations

– Continuous spatial variations in tallies

- **MCNP5**
  - **Overview**
  - **New features**
  - **Creation & installation**
- **Parallel calculations**
  - **ASC teraflop systems**
  - **Linux clusters**
  - **Parallel demo**
- **Nuclear data**
  - **ENDF66**
  - **ACTI**
  - **SAB2002**
  - **Temperature-specific libraries (DOPPLER code)**
  - **Criticality validation suite**

- **Improvements & enhancements in progress**
  - **Eigenvalue calculations**
    - **Stationarity detection**
    - **Dominance ratio**
  - **Effects of source shape changes on perturbations**
  - **Automated Variance Reduction: MCNP5 + deterministic adjoint**
  - **Continuously varying tallies**
  - **ENDF/B-VII nuclear data libraries**

MCNP5

Forrest Brown, Tom Booth , Jeffrey Bull, Art Forster,
Tim Goorley, Grady Hughes, Russell Mosteller, Richard Prael,
Elizabeth Selcow, Avneet Sood, Jeremy Sweezy

- **For more than 25 years, MCNP & its data libraries have been developed and supported by the Monte Carlo team in X-Division (and its predecessors).**

- **Diagnostics Applications Group (X-5)**
  - **11 MCNP code developers in X-5**
  - **Physical Data team also in X-5**
  - **Two application teams in X-5**

- **Work is funded by:**
  - **US DOE ASC Program**
    - **Advanced Simulation & Computing**
  - **US DOE Criticality Safety Program**

- **Continued strong support for MCNP provides funding for R&D activities in many diverse areas of Monte Carlo methods**

1940s   1977   2004
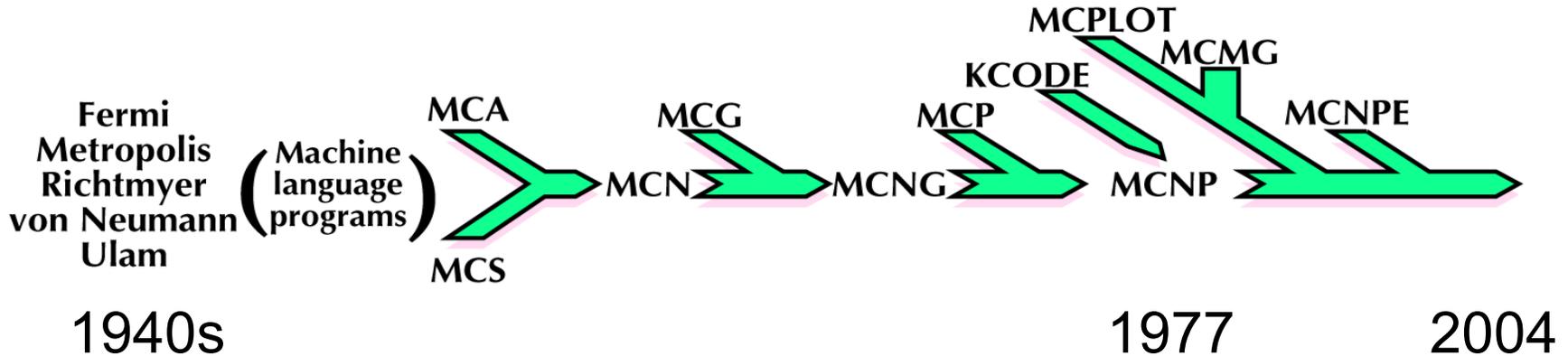
Monte Carlo transport of neutrons, photons, & electrons

- **Particles**
    - **Neutrons, n:** 10^{-5} eV - 150 MeV
    - **Photons, p:**   1 KeV - 100 GeV
    - **Electrons, e:**   1 KeV - 1 GeV

    - **Single particles:**   n, p, e
    - **Coupled calculations:** n/p, n/p/e, p/e, e/p
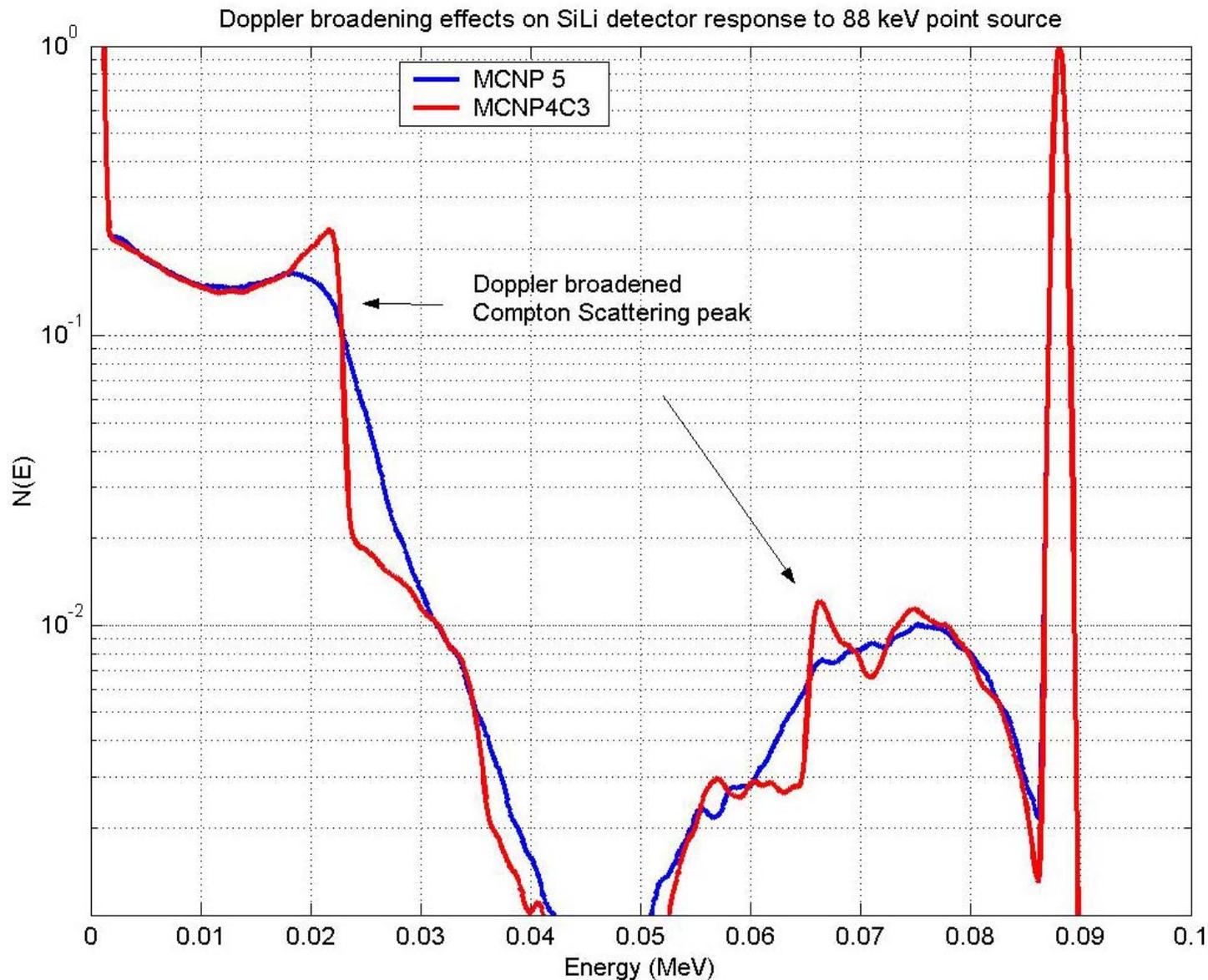- **General 3D geometry**
- **Continuous-energy physical data**
- **Many code options: Keff, detectors, variance reduction, tallies, …**

Modernization of MCNP

During 2001-2002, every line of MCNP coding was reworked to produce MCNP5

- Conversion to ANSI-Standard Fortran-90

- Emphasis on code readability & ease of future development

- Standard parallel coding: MPI (message-passing) + OMP (threads)

- Vastly improved modern coding style

- Fortran-90 dynamic memory allocation

- Completely new installation system

- New features & new physics

- New cross-section data libraries

- Extensive SQA and V&V

– **New cross-section data libraries**

– **Updated MCNP Users Manual – 1,000 pages**

– **Doppler energy broadening for photon transport**

– **Extended random number package**

– **Improved parallel processing**

– **Mesh tallies**

– **Image tallies, radiographs**

– **Sources: translate/rotate/repeat, Gaussian, particle type**

– **Easier specification of sources in repeated structures**

– **Time & energy splitting/rouletting**

– **Unix-based build system, using GNU make**

– **Plotting improvements**

Doppler Energy Broadening for Photons

Doppler broadening effects on SiLi detector response to 88 keV point source

- MCNP 5
- MCNP4C3

Doppler broadened Compton Scattering peak

New Data Libraries
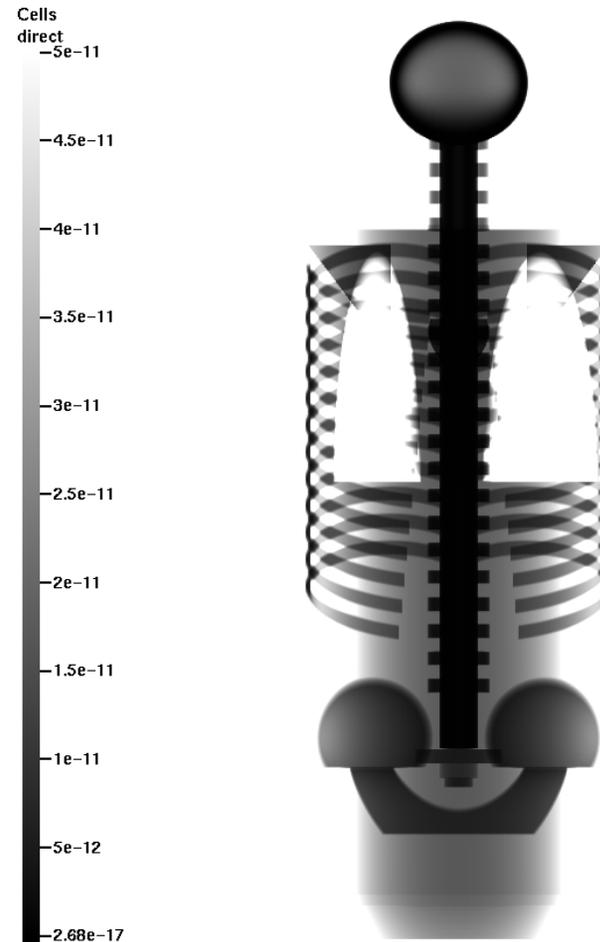
- **New data libraries released by X-5 Data Team**
  - **ENDF66**: Based on ENDF/B-VI, Release 6
  - **ACTI**: Based on ENDF/B-VI, Release 8
  - **SAB2002**: Improved evaluations for thermal scattering
  - **MCPLIB03** & **MCPLIB04**: New photoatomic data libraries

- **ENDF66**
  - **173 nuclides**, compared with 122 nuclides for ENDF60
  - Smaller NJOY processing tolerance, 0.001 instead of ~0.005
  - Probability tables, charged-particle production, delayed neutron data
  - Tabular angular distributions

- **ACTI**
  - MCNP data for prompt gamma-ray spectroscopy, includes **41 nuclides**
  - Advanced Computational Technology Initiative (ACTI) CRADA

- **SAB2002**
  - Based on ENDF/B-V1.3
  - Data for **15 moderators**, includes more secondary energies and angles

Neutral Particle Image Tallies

- **Neutron and photon radiography uses a grid of point detectors (pixels)**

- **Each source and collision event contributes to all pixels**

MCNP Model of Human Torso

Simulated Radiograph – 1 M pixels

Cells direct

- 5e-11
- 4.5e-11
- 4e-11
- 3.5e-11
- 3e-11
- 2.5e-11
- 2e-11
- 1.5e-11
- 1e-11
- 5e-12
- 2.68e-17

New Edits of Crit-Safety Parameters

_____

the final estimated combined collision/absorption/track-length keff = 0.87964
   with an estimated standard deviation of 0.00256

the estimated 68, 95, & 99 percent keff confidence intervals are
   0.87708 to 0.88221, 0.87455 to 0.88474, and 0.87288 to 0.88641

the final combined (col/abs/tl) prompt removal lifetime = 7.7675E-05 seconds
   with an estimated standard deviation of 4.0076E-07

the average neutron energy causing fission = 1.5970E-01 mev
the energy corresponding to the average neutron lethargy causing fission = 1.9432E-07 mev

the percentages of fissions caused by neutrons in the
   thermal, intermediate, and fast neutron ranges are:
   (<0.625 ev): 85.90 %   (0.625 ev – 100 kev): 8.53 %   (>100 kev): 5.57%

the average fission neutrons produced per neutron absorbed (capture + fission)
   in all cells with fission = 1.5837E+00
the average fission neutrons produced per neutron absorbed (capture + fission)
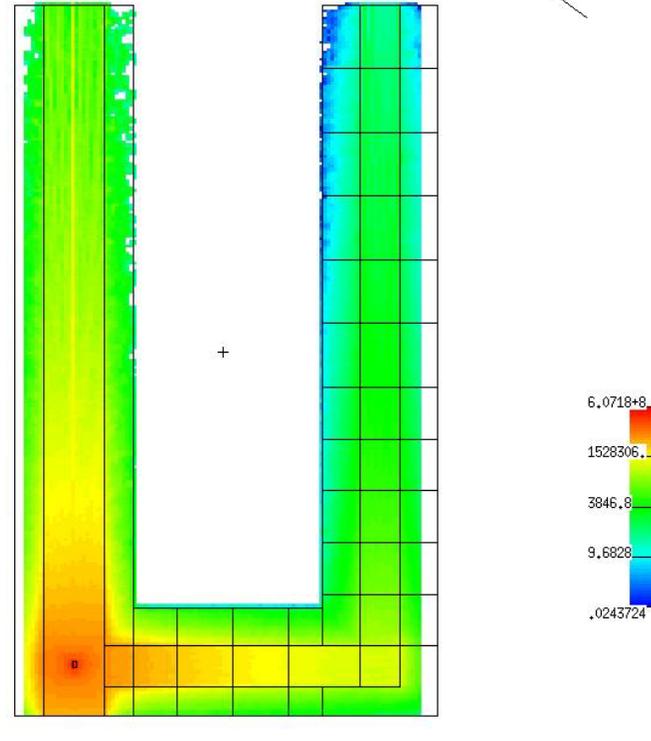   in all the geometry cells = 8.8306E-01

the average number of neutrons produced per fission = 2.442
_____

- Traditional MCNP tallies are for cells, surfaces, or points
- Now, an arbitrary mesh for tallies can be superimposed on the MCNP5 problem geometry

Problem geometry
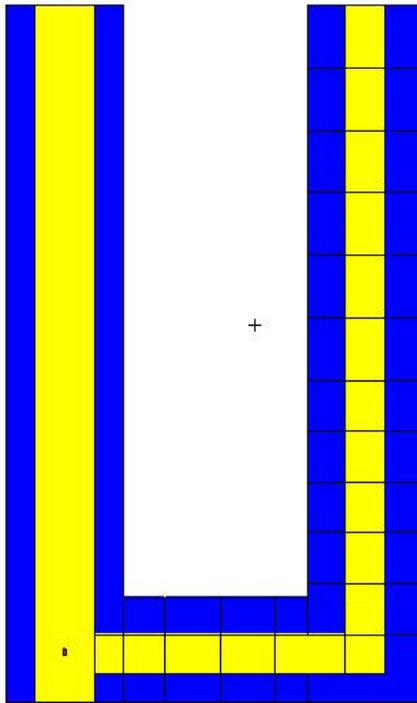
Flux plot from mesh tally

6.0718+8
1528306.
3846.8
9.6828
.0243724

- **FMESH card -- Specify meshes for tallies**
  - XYZ or cylindrical
  - Totally independent of the real problem geometry
  - Specify coarse mesh bounds & number of fine-mesh subdivisions for   X, Y, Z, E   or   R, Z, Θ, E
  - Does not have to cover entire problem
  - Can have any number of meshes for separate tallies
  - Separate meshes can overlap or be disjoint
  - Other cards to modify mesh tallies: **DE, DF, FM**
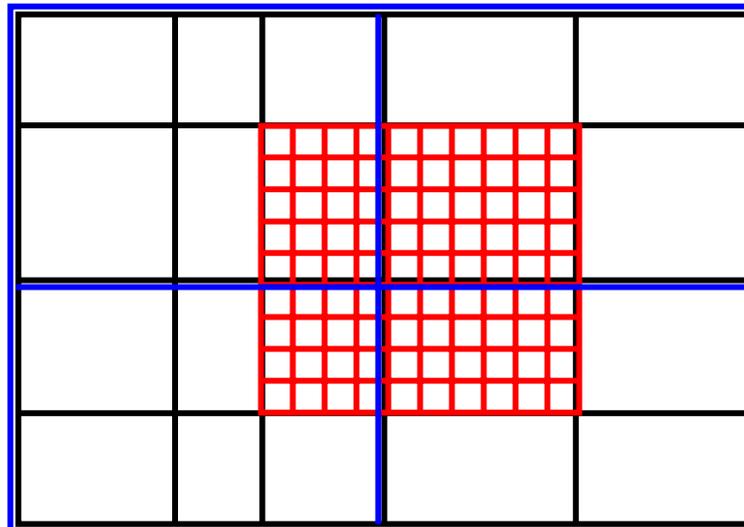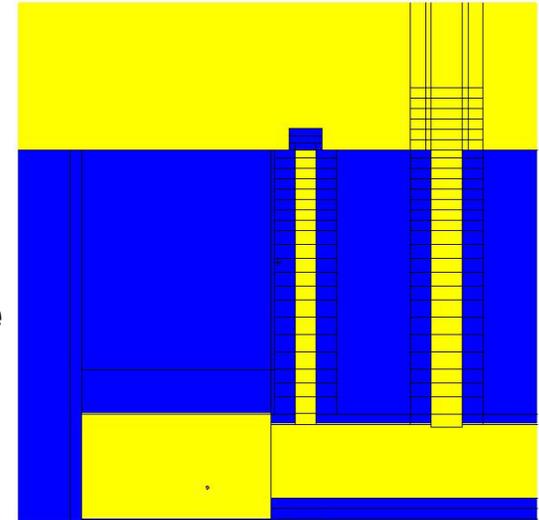
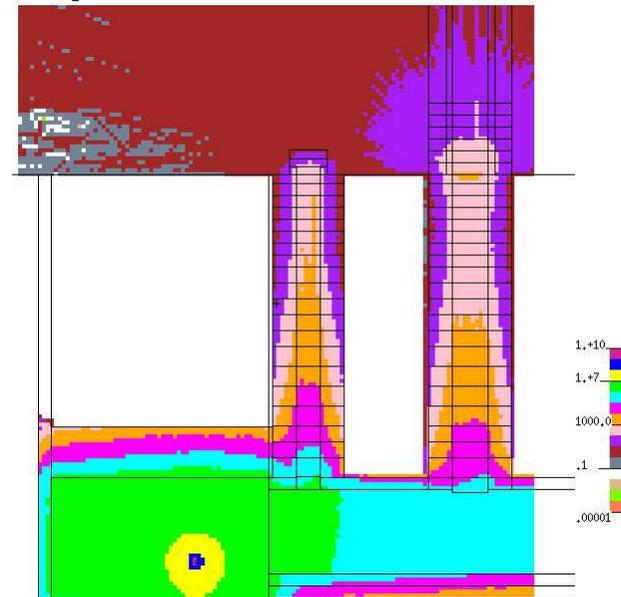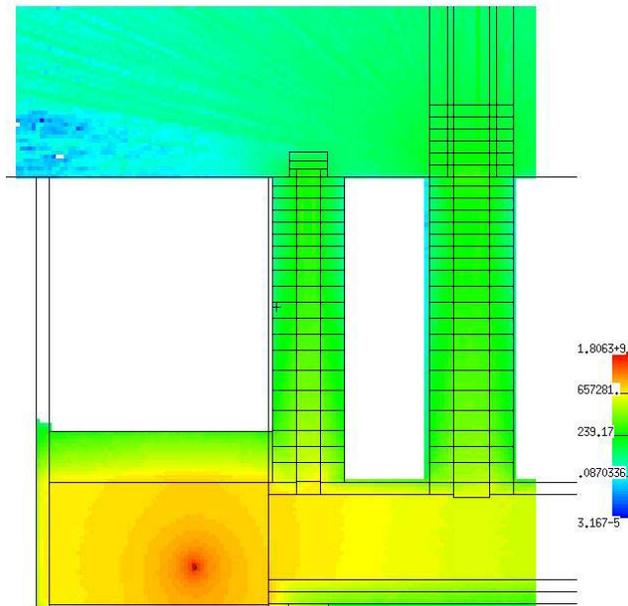# **Proton Storage Ring**
at LANSCE accelerator

Geometry
Blue = concrete
Yellow = air

Dose rate calculation for cable penetrations

- Fuel storage vault - fission distribution
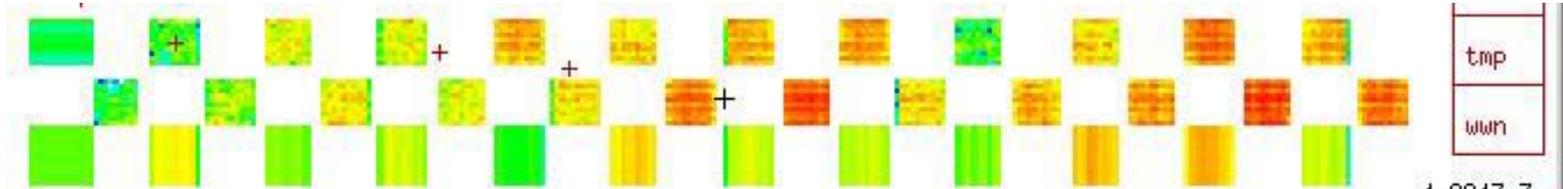
- Detail

Computer Systems Supported
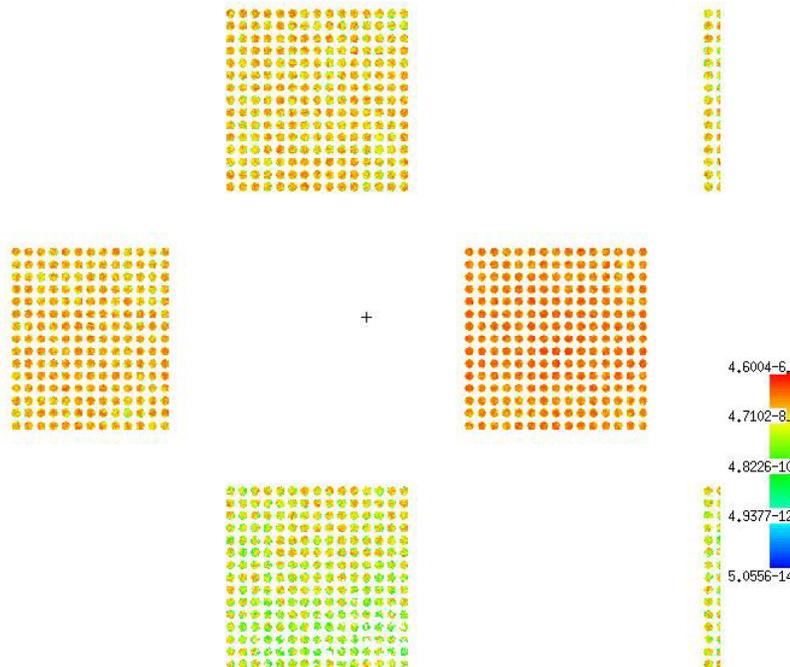
Serial & parallel (MPI, OMP, MPI/OMP, PVM, PVM/OMP):

- **Unix systems**
  - **SGI IRIX64**
  - **IBM AIX**
  - **HP/Compaq OSF1**
  - **Sun SunOS**

Serial & parallel (MPI, PVM):

- **Linux systems**
  - **with Absoft compiler**
  - **with Lahey compiler**
  - **with Intel compiler**
  - **with Portland Group compiler**
  - **with NAG compiler**
- **Mac OS X systems**
  - **with Absoft compiler**
  - **with IBMXL compiler**

Serial & parallel (MPI, PVM):

- **Windows PC systems**
  - **with CVF compiler**
  - **with Absoft compiler**
  - **with Lahey compiler**
  - **with Intel compiler**

- **Itanium systems**
  - **with Intel compiler**

X11 graphics – all systems

www-xdiv.lanl.gov / x5 / MCNP

- **Has all recent LA-UR reports & publications:**
  - New version of criticality primer (~200 pages):
    "**Criticality Calculations with MCNP5 - A Primer**", LA-UR-04-0294

  - "**MCNP — A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory**",   LA-UR-03-1987

  - "**Bibliography of MCNP Verification & Validation: 1990-2003",** LA-UR-03-9032

  - All **Ueki/Brown papers** on k-effective calculations: correlation effects, stationarity diagnostics, dominance ratio, etc.

  - "**MCNP5 Parallel Processing Workshop**", LA-UR-03-2228, parallel Monte Carlo, Linux clusters, Windows clusters

  - … and many more

- **MCNP5 updates & patches**
- **Schedule for upcoming MCNP5 classes**

- **Manual**

  MCNP — A General Monte Carlo N-Particle Transport Code, Version 5

Volume I:	**Overview and Theory**,	LA-UR-03-1987
Volume II:	**Users Guide,**	LA-CP-03-0245
Volume III:	**Developers Guide,**	LA-CP-03-0284

  - Volume I - Theory is on the MCNP website
  - Volumes I, II, & III are included with the code package from RSICC

- **MCNP5 code package**

  - April 2003 - Initial release from RSICC: **www-rsicc.ornl.gov**
  - European users:
    - The traditional exchange agreement between RSICC & OECD/NEA Data Bank expired and is **still** being negotiated.
    - For now, request the code from RSICC

- **Patches**

  - Nov 2003 - Patch
    - Bug fixes (surface area, files with MPI, …)
  - May 2004 - Patch
    - NPS up to ~10^{19}
    - Speedup for lattice tallies
    - Bug fixes (restarts, DXTRAN in repeated structures, …)

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Demonstration of MCNP5 Installer
for Windows PCs

Demonstration of MCNP5 compile
on Unix system (Mac OS X)

Parallel Computing

Forrest Brown, Tim Goorley, Jeremy Sweezy,

Susan Post, Richard Barrett

See "MCNP5 Parallel Processing Workshop", LA-UR-03-2228, FB Brown, JE Sweezy, JT Goorley (2003) on the MCNP website

Advanced Simulation & Computing – ASC
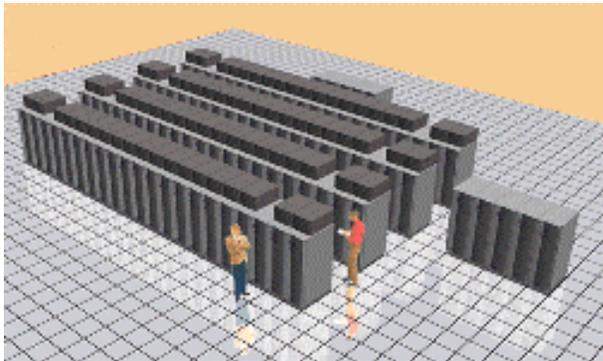
Red – 3 TeraOps

Blue Pacific – 3 TeraOps

Blue Mountain – 3 TeraOps

White – 12 TeraOps

ASC™

Q – 20 TeraOps

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- Use **message-passing** to distribute work among slaves ("boxes")
- Use **threading** to distribute histories among individual cpus on box

MPI

OpenMP
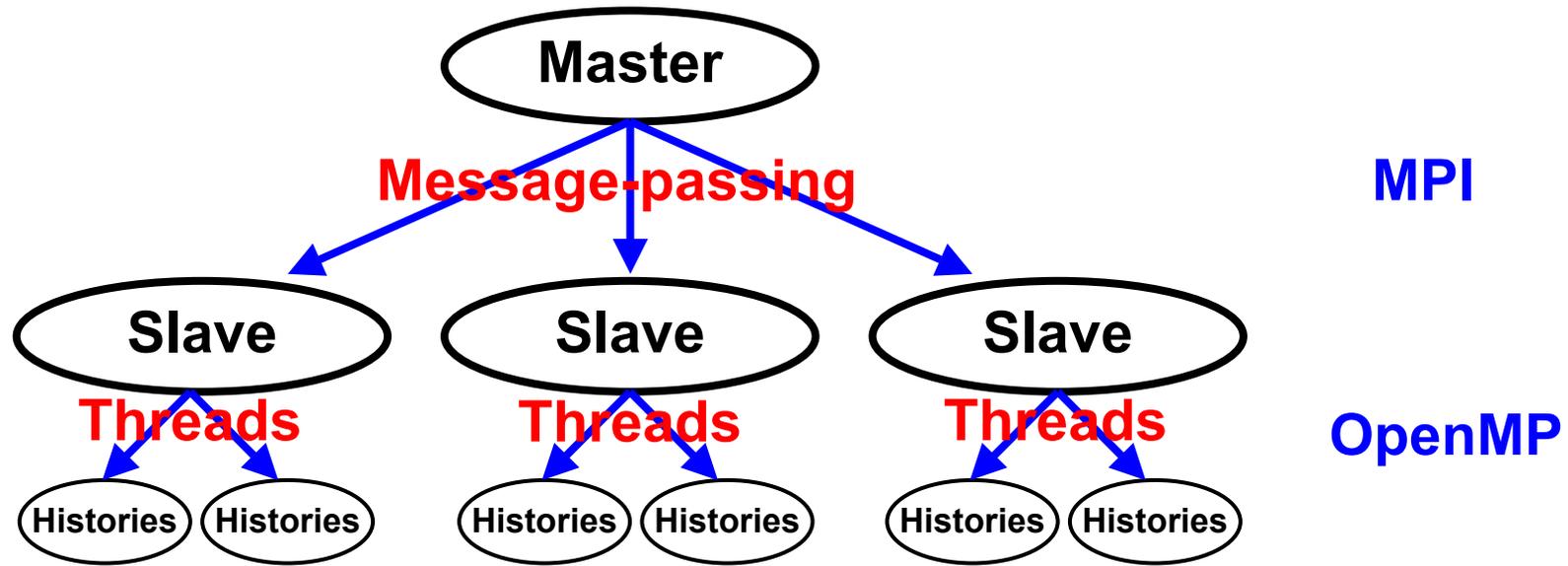
- **We routinely test MCNP5 on:**
    - **ASCI Bluemountain –** SGI, 48 boxes x 128 cpus/box
    - **ASCI White –** IBM, 512 boxes x 16 cpus/box
    - **ASCI Q –** HP, 2 x 512 boxes x 4 cpus/box
    - **Linux clusters**
    - **Windows PC cluster**
- **1,000 processor jobs are "routine"**

Load Balancing & Fault Tolerance

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Each arrow: same # histories

Repeat…

M

S   S   S

Fast CPU
Medium CPU
Slow CPU

Control   Compute   Rendezvous
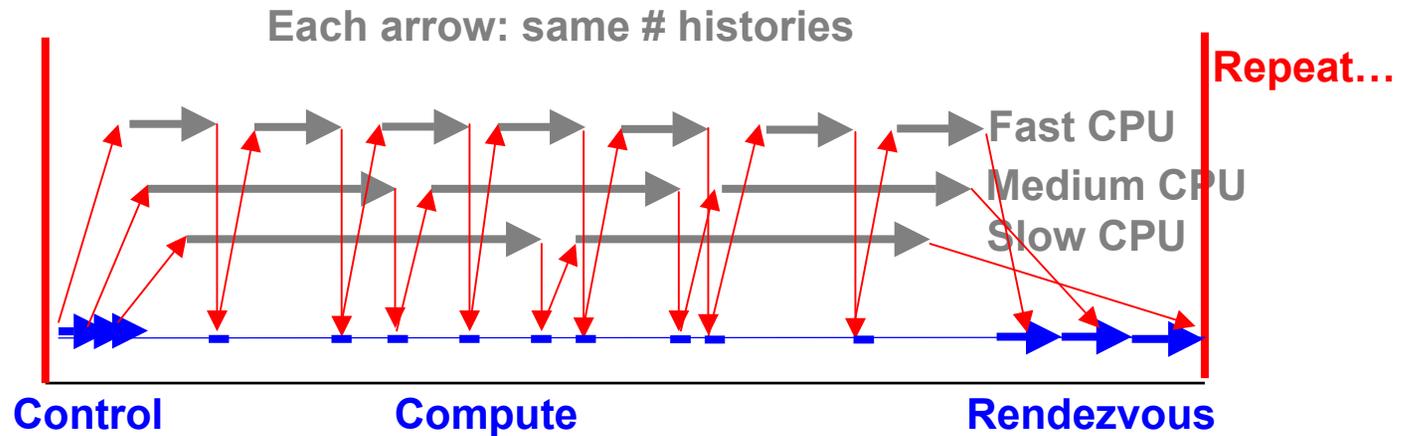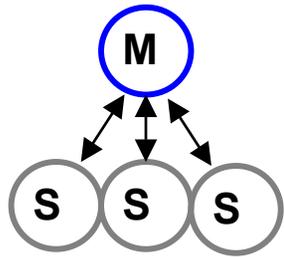
- **Load balancing:**   Self-scheduling of histories on slaves

- **Fault tolerance:**   Periodic rendezvous to save restart files

- **Parallel efficiency:** [compute time] / [compute + rendezvous time]

Parallel MC Performance Scaling

T_S T_C T_R

M

S   **S**   **S**

Repeat…

Control   **Compute**   **Rendezvous**
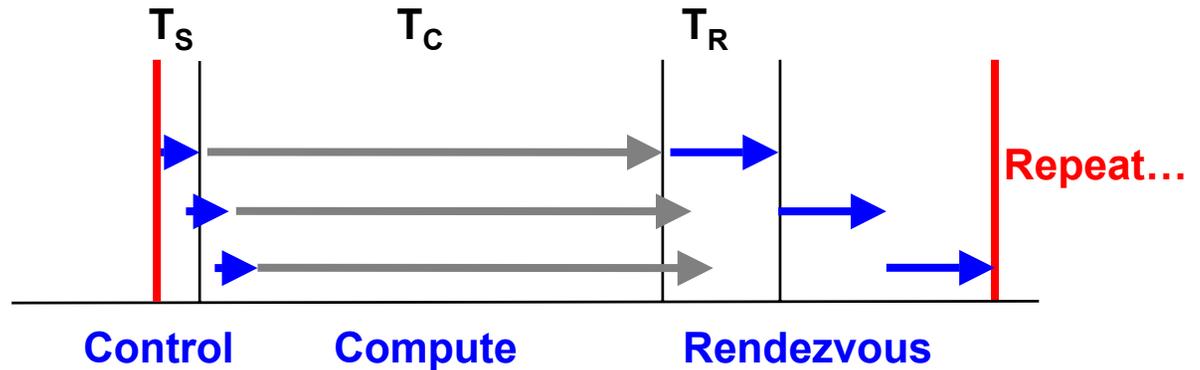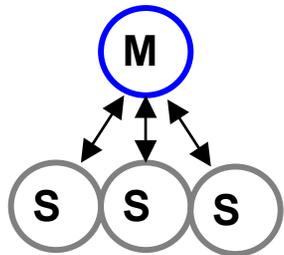
N = # processors

T_1 = CPU time for M histories using 1 processor

       (Depends on physics, geometry, compiler, CPU speed, memory, etc.)

L   = amount of data sent from 1 slave each rendezvous

$T_S = 0$ negligible, time to distribute control info

$T_R = s + L/r$ **s** = latency for message,   **r** = streaming rate

$T_C^{fix} = T_1 / N$ fixed problem size, **M** histories/rendezvous

$T_C^{scale} = T_1$ scaled problem size, **NM** histories/rendezvous

Parallel MC Performance Scaling

- **Scaling models, for master/slave with serial rendezvous**

    - "fixed"   = constant number of histories/rendezvous, M   **(constant work)**
    - "scaled"   = M histories/slave per rendezvous, NM total   **(constant time)**

Hist./rendezvous	**Speedup**
fixed	$S = N / (1 + cN^2)$
scaled	$S = N / (1 + cN)$
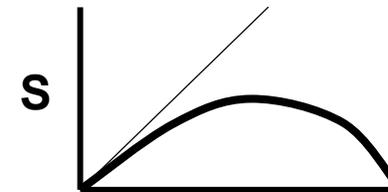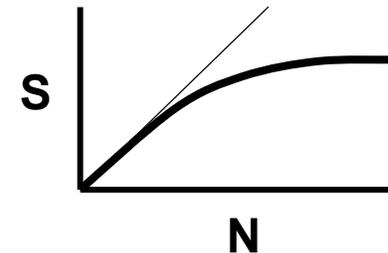
N = number of slaves
$c = (s + L/r) / T_1$

$T_1 \sim M$,   more histories/rendezvous ➔ larger T_1 , smaller c
S+L/r,   fixed, determined by number of tallies, ….

As M➔infinity, c➔0,   S➔N   (limit for 1 rendezvous)

Parallel MC Summary

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- **Master/slave algorithms work well**

  - Load-balancing: Self-scheduling

  - Fault-tolerance: Periodic rendezvous

  - Random numbers: Easy, with LCG & fast skip-ahead algorithm

  - Tallies: Use OpenMP "critical sections"

  - Scaling: Simple model, more histories/slave + fewer rendezvous

  - Hierarchical: Master/slave MPI, OpenMP threaded slaves

  - Portability: MPI/OpenMP, clusters of anything

- **Remaining difficulties**

  - Memory size: Entire problem must fit on each slave

   - Domain-decomposition has had limited success
      - Should be OK for reactor problems
      - Does not scale well for shielding or time-dependent problems
      - For general 3D geometry, effective domain-decomposition is unsolved problem
    - Random access to memory distributed across nodes gives huge slowdown
      - May need functional parallelism with "data servers"

MCNP5 Parallel Scaled Speedup
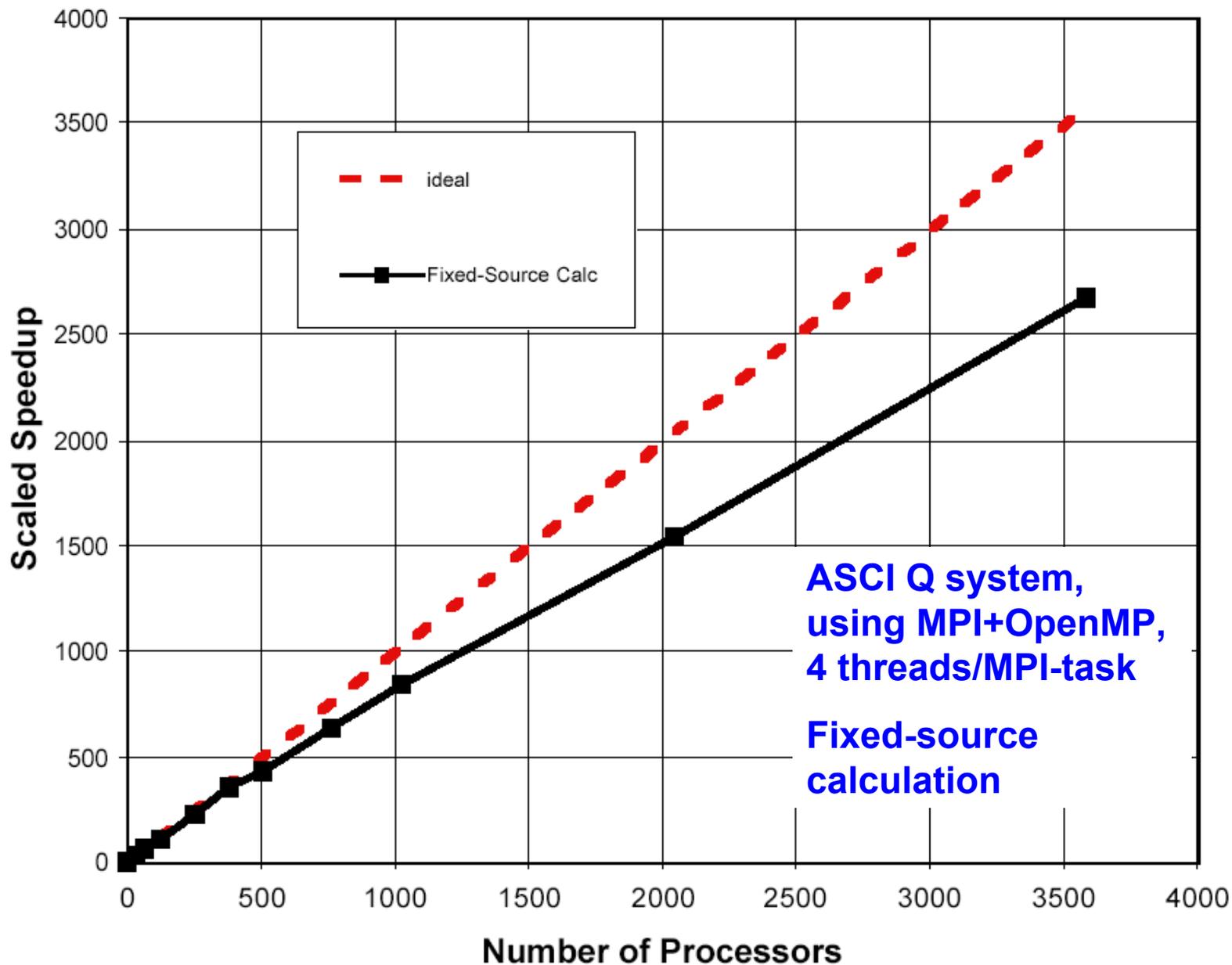
MCNP Speed vs. Number of Processors
BNCT Model w/ NPS=100,000 on a Linux Cluster w/ MPICH
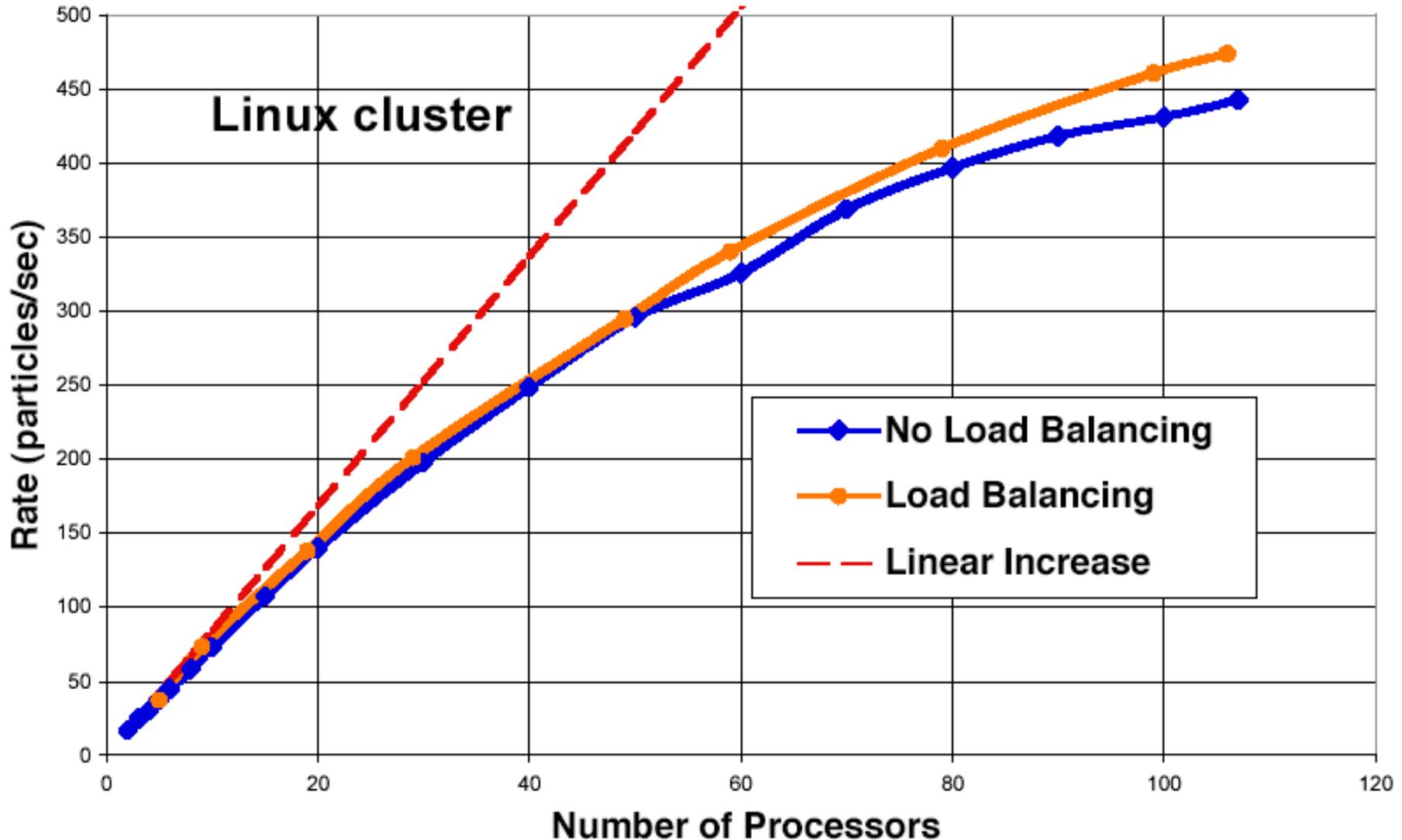
- **Stability**

- **Flexibility**

- **Linux supports almost all hardware**

- **Commercial and free distributions of Linux OS**

- **Large user community**

- **Network booting capability**

- **Supports various types of network file systems (NFS, PVFS, etc)**

- **Cost**

Linux Clusters - Topology

Internet/LAN

eth0 Internet IP

Master

Second Master

Optional

eth1 172.31.0.1

Network Switch

Storage or Backup

| Slave 1 172.31.0.2 | Slave 2 172.31.0.3 | Slave 3 172.31.0.4 | Slave 4 172.31.0.5 | Slave 5 172.31.0.6 | Slave 6 172.31.0.7 |
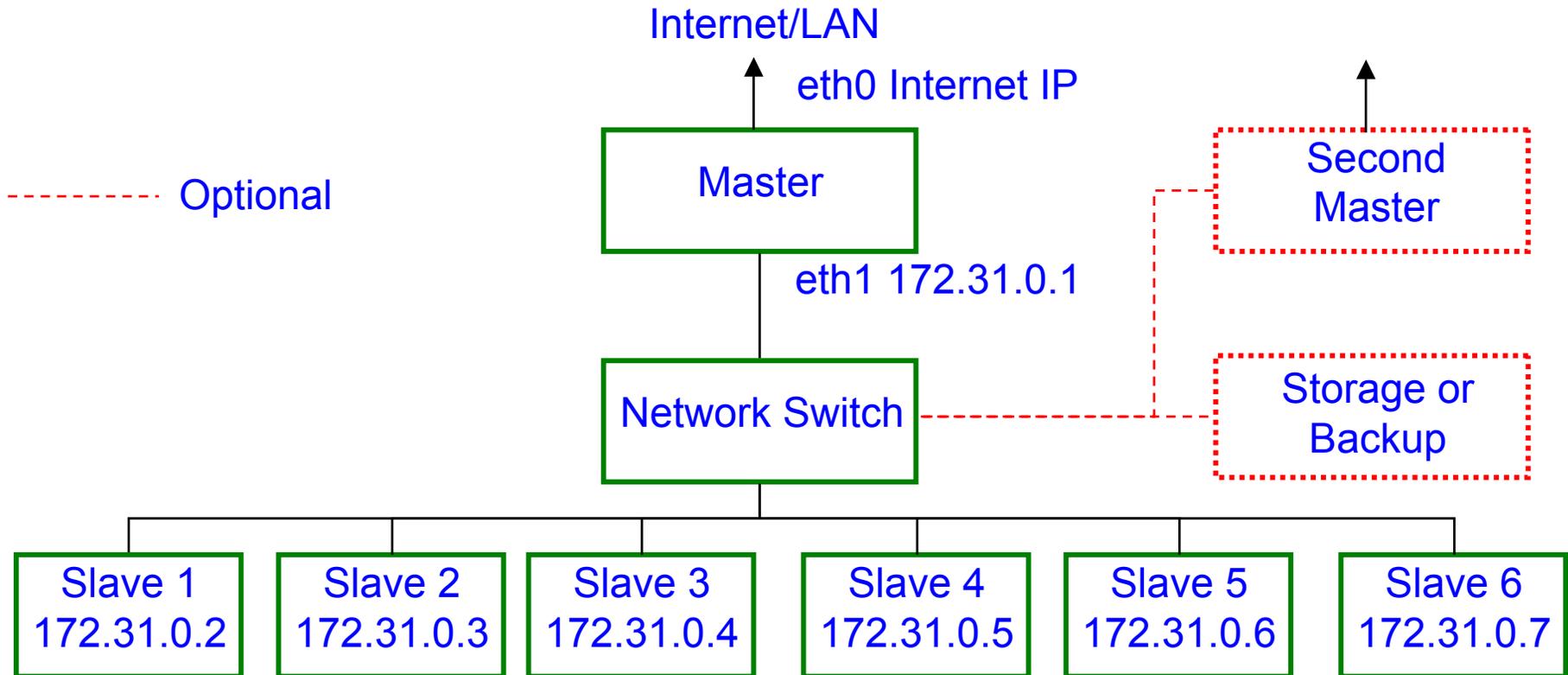
Private IP Addresses:

- The Internet Assigned Numbers Authority (IANA) has reserved the following three blocks of the IP address space for private internets:
  - 10.0.0.0   - 10.255.255.255
  - 172.16.0.0   - 172.31.255.255
  - 192.168.0.0   - 192.168.255.255

31

Clustering Software:

- Scyld Beowulf (www.scyld.com) (www.linuxcentral.com has Scyld CD for $2.95 w/o support)

- NPACI Rocks (www.rocksclusters.org)

- OSCAR (oscar.sourceforge.net)

- Do-it-yourself
  - Standalone Slaves
  - Diskless Slaves

Job Scheduling Software:

- Maui Scheduler (www.supercluster.org/maui)

- OpenPBS (www.openpbs.org)

- PBSPro (www.pbspro.com)

- LSF   (www.platform.com)

Diskless Linux Clusters

- **Advantages**
  - Easy setup
  - Little maintenance required for the slaves nodes.
  - Slave nodes can be added and replaced rapidly.
  - Ad-hoc clusters can be assembled rapidly.
  - Reduced cost of slaves.

- **Disadvantages**
  - Complete operating system resides on the network (slower).
  - No local disk for swap space.
  - Complete cluster reliant on the master.

To Build a Diskless Linux Cluster you need:

1. One computer as the master host running Linux

- Linux operating system
- Two network cards (only one required if no external network)
- Video card
- Monitor and keyboard
- Hard drives
- CD-ROM and Floppy drives

2. Some type of network

- Network hub or network switch

3. One or more computers as slaves

- One network card per slave
- No hard drive required
- No operating system required
- Video card
- CD-ROM or Floppy drives

4. Optional

- KVM switch

Diskless Linux Clusters

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Building a Diskless Linux Cluster Overview:

1. Create slave boot media
   - Build Linux kernel for the slaves
   - Install and configure boot loader (syslinux) on a floppy or CD.
   - Install Linux kernel on to the floppy or CD.

2. Create slave file system

3. Configure NFS and security

4. Connect the slaves to the master and boot

Build a kernel for the Diskless Slaves:

1. Download latest Linux kernel (www.kernel.org)

2. Unpack in `/usr/src/linux`

3. `% make mrproper; make xconfig`

4. Select the following options to be build into the linux kernel.

   1. Networking options ---> IP: kernel level autoconfiguration
   2. File Systems ---> Network File Systems ---> NFS file system support ---> NFS file system support
   3. File Systems ---> Network File Systems ---> NFS file system support ---> Root over NFS
   4. Block devices ---> Loopback device support
   5. Network device support ---> Ethernet (10 or 100 Mbit) ---> Select your network cards

5. `% make dep; make bzImage`

6. The new kernel resides at
   `% /usr/src/linux/arch/i386/boot/bzImage`

Diskless Linux Clusters

Diskless Linux Clusters

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Create slave boot media:

1. Insert a disk into the CD-RW drive and run:

    ```
    % syslinux -s /dev/fd0
    ```

2. Edit the file `syslinux.cfg`
    (note that the "append" line shown here as 3 lines is really 1 long line)

    ```
    default linux
    append init=/sbin/init root=/dev/nfs
        ip=172.31.0.2:172.31.0.1:172.31.0.1:255.255.255.0:slave1:e
        th0:'bootp' nfsroot=172.31.0.1:/tftpboot/172.31.0.2
    Say Remote Booting Slave1
    Say Slave1 IP Address = 172.31.0.2
    ```

3. Copy the linux kernel to the CD and rename to "linux"

    ```
    % cp /usr/src/linux/arch/i386/boot/bzImage /mnt/floppy/linux
    ```

Create first slave node file system:

1. On the master node
```
% mkdir /tftpboot; cd /tftpboot
```

2. Download and run the `nfsrootinit` script to create the first root file system. (http://etherboot.sourceforge.net/doc/html/nfsrootinit.txt)
```
% chmod u+x nfsrootinit.txt
% ./nfsrootinit.txt 172.31.0.2
```

3. Edit `/tftpboot/172.31.0.2/etc/fstab` to mount the correct directories via NFS.
```
None    /dev/pts    devpts      gid=5,mode=620  0 0
None    /proc       proc        defaults        0 0
None    /dev/shm    tmpfs       defaults        0 0
172.31.0.1:/tftpboot/172.31.0.2 /       nfs rw,soft,rsize=8192,wsize=8192,intr
172.31.0.1:/home                /home   nfs rw,soft,rsize=8192,wsize=8192,intr
172.31.0.1:/usr                 /usr    nfs rw,soft,rsize=8192,wsize=8192,intr
```

4. Edit `/tftpboot/172.31.0.2/sysconfig/network` and change the `HOSTNAME` variable.
```
HOSTNAME="slave1.mcnpengine.lanl.gov"
```

Duplicate slave node file system for other slaves:

1. Download and run the `nfsrootdup` script to duplicate the first root file system. (http://etherboot.sourceforge.net/doc/html/nfsrootdup.txt)

   ```
   % chmod u+x nfsrootinit.txt
   % ./nfsrootinit.txt 172.31.0.2 172.31.0.3
   ```

2. Edit `/tftpboot/172.31.0.3/etc/fstab` to mount the correct directories via NFS.

   ```
   None    /dev/pts    devpts      gid=5,mode=620  0 0
   None    /proc       proc        defaults        0 0
   None    /dev/shm    tmpfs       defaults        0 0
   172.31.0.1:/tftpboot/172.31.0.3 /       nfs rw,soft,rsize=8192,wsize=8192,intr
   172.31.0.1:/home                /home   nfs rw,soft,rsize=8192,wsize=8192,intr
   172.31.0.1:/usr                 /usr    nfs rw,soft,rsize=8192,wsize=8192,intr
   ```

3. Edit `/tftpboot/172.31.0.3/sysconfig/network` and change the `HOSTNAME` variable.

   ```
   HOSTNAME="slave2.mcnpengine.lanl.gov"
   ```

Set up the NFS Server and Security:

1. Edit /etc/exports
```
/home       172.31.0.0/255.255.255.0(rw,no_root_squash)
/usr        172.31.0.0/255.255.255.0(rw,no_root_squash)
/tftpboot
172.31.0.0/255.255.255.0(rw,no_root_squash,no_subtree_check)
```

2. Start or restart the NFS server. On a Redhat system use:
```
% /etc/init.d/nfs start
```
or
```
% /etc/init.d/nfs restart
```

3. Add the slaves hosts to your /etc/hosts file
```
172.31.0.2      slave1.mcnpengine.lanl.gov         slave1
172.31.0.3      slave2.mcnpengine.lanl.gov         slave2
172.31.0.4      slave3.mcnpengine.lanl.gov         slave3
172.31.0.5      slave4.mcnpengine.lanl.gov         slave4
172.31.0.6      slave5.mcnpengine.lanl.gov         slave5
```

4. Edit /etc/hosts.allow and add the following line
```
all : 172.31.0.
```

5. If the master is connected to an external network use a firewall (iptables or ipchains) to block access to all but a limited number of privileged ports.

Linux Clusters – Information

- **Books**
  - "Linux Clustering: Building and Maintaining Linux Clusters" Charles Bookman
  - "Beowulf Cluster Computing with Linux" Thomas Sterling, Editor

- **Websites**
  - www.beowulf.org
  - www.beowulf-underground.org

- **HOWTOs** (http://www.tldp.org/)
  - Beowulf-HOWTO
  - Linux Cluster HOWTO
  - Diskless Nodes HOWTO
  - Root over NFS Clients & Server HOWTO
  - Root over NFS - Another Approach HOWTO
  - Network Boot and Exotic Root HOWTO
  - NFS-Root-Client Mini-HOWTO
  - NFS-Root Mini-HOWTO

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**Diagnostics
Applications
Group (X-5)**

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Demo of MCNP5
on a diskless laptop cluster
running Linux

1. Boot master node.
2. Boot slave nodes.
3. Verify network using ping.

MCNP5 Linux Parallel Calculations

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**Diagnostics
Applications
Group (X-5)**

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- **Dual CPU Desktop Timing Study**
  - Dual 2.2GHz Intel Pentium IV XEON CPUs, 1 GB RAM, 512k L2 cache, running Linux 2.4.20 kernel and Redhat Linux 7.3 distribution

Wall Clock Runtimes	Sequential	PVM tasks 2	PVM tasks -2	MPI -np 3	MPI -np 3 balance
NPS 10,000	9:41	6:09	5:12	5:21	5:11
NPS 100,000	100:49	58:42	49:32	52:14	48:49

Using:
- Type 1 cross sections
- MPICH 1.2.5 compiled with --enable-yield=sched_yield
- PVM 3.4.4

MCNP5 Linux Parallel Calculations

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**Diagnostics
Applications
Group (X-5)**

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MCNP Speed vs. Number of Processors
BNCT Model w/ NPS=10,000 on a Linux Cluster w/ MPICH
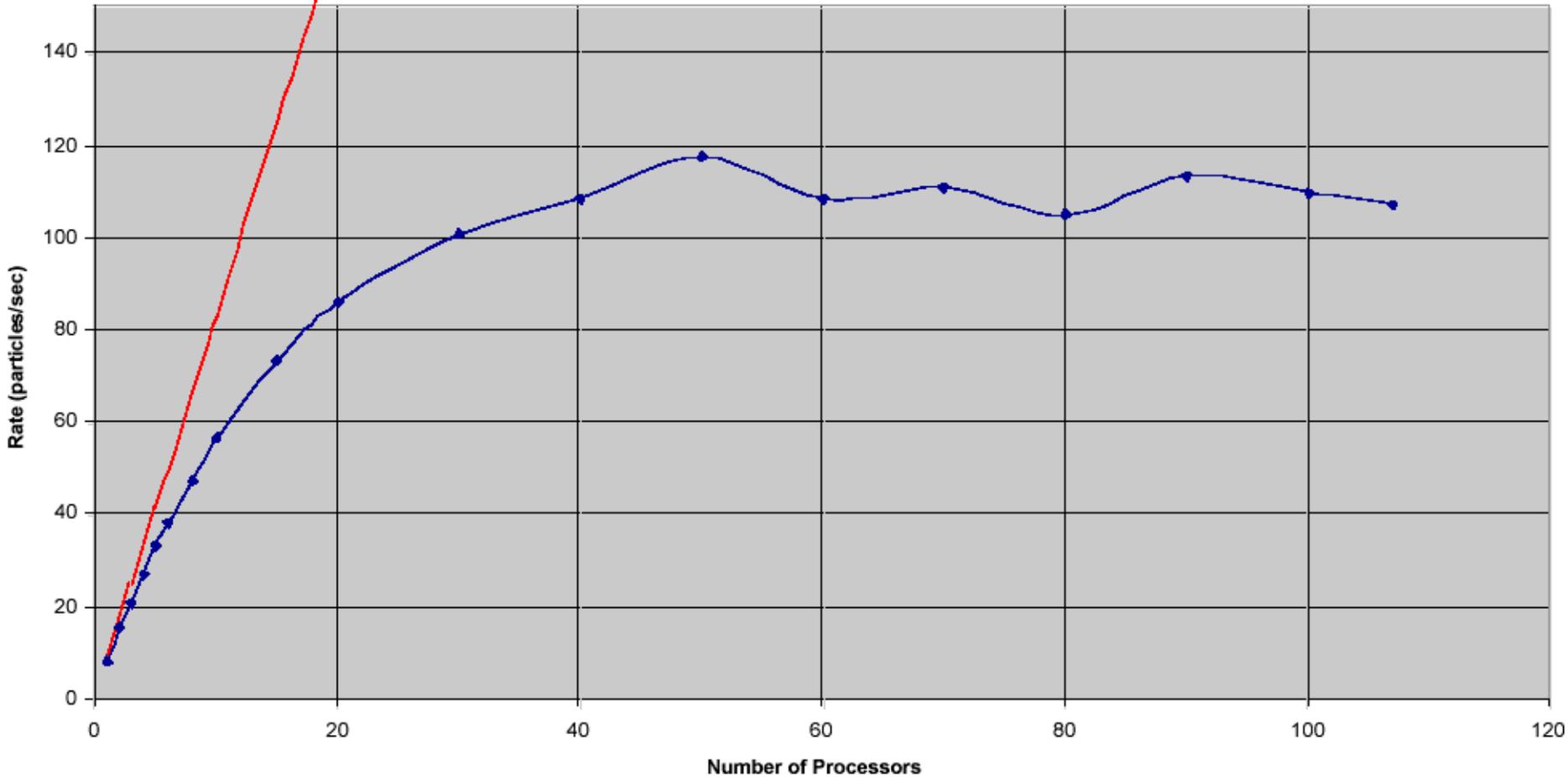
MCNP Speed vs. Number of Processors
BNCT Model w/ NPS=100,000 on a Linux Cluster w/ MPICH

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Diagnostics
Applications
Group (X-5)

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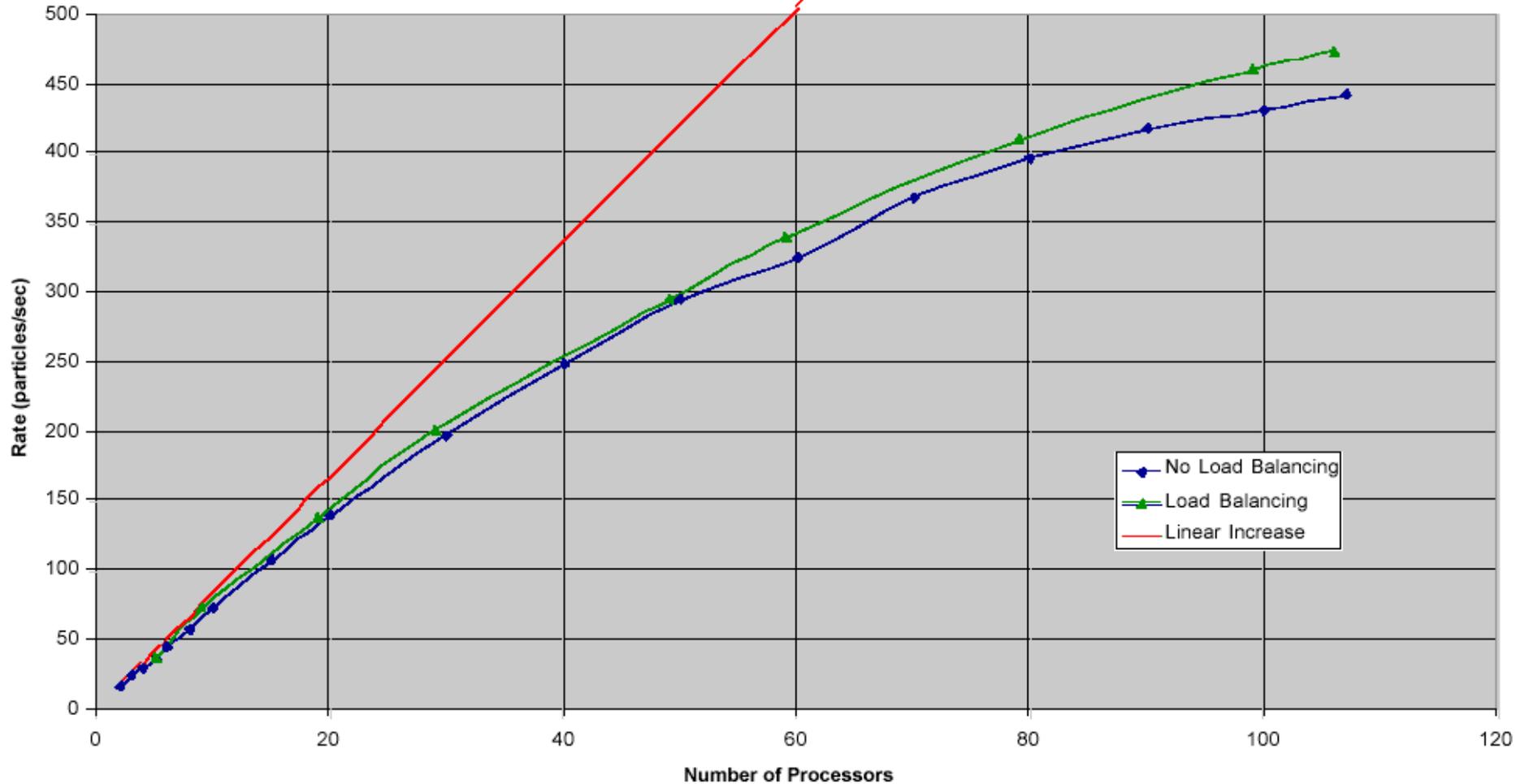
TOPICS TO BE DISCUSSED

Validation suites for MCNP
    Criticality
    Radiation shielding

Nuclear data libraries for MCNP
    ENDF/B-V
    ENDF60
    ENDF66
    ENDF/B-VI (Final release)

Forthcoming improvements in nuclear data (preliminary ENDF/B-VII)

Temperature-specific nuclear data libraries and the DOPPLER code

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VALIDATION SUITES FOR MCNP

MCNP Workshop
PHYSOR 2004
April 25, 2004

MCNP INSTALLATION TEST SUITE

MCNP distribution package includes installation ("regression") test suite

Cases have been constructed to test input options and to execute quickly

Many of the cases are physically unrealistic

Results are not well converged

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MCNP VALIDATION SUITES

Validation suites are being developed and tested for specific types of applications

Objectives are to (1) provide true validation of the MCNP package (including nuclear data) and (2) to establish a basis for assessing the impact of future improvements to MCNP and of changes to its associated nuclear data libraries

All cases in the suites are based on experimental benchmarks

Currently, validation suites exist for criticality and radiation-shielding applications

Input files for the cases in the validation suites soon will be available on the MCNP website, along with reference results from MCNP5 using the ENDF/B-VI nuclear data library and 1,000,000 active histories for each case

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COMPUTER RESOURCE REQUIREMENTS
FOR VALIDATION SUITES

(1,000,000 active histories per case)

Computer	SGI Supercomputer	Pentium-III PC	Pentium-4 PC
Operating system	IRIX64*	Windows 2000	Windows 2000
Clock speed	400 MHz	800 MHz	1400 MHz
Memory (RAM)	—	256 MB	512 MB
Criticality suite	18.7 CPU Hours	16.3 CPU Hours	10.8 CPU Hours
Radiation-shielding suite	6.6 CPU Hours	5.9 CPU Hours	4.4 CPU Hours
Total	25.3 CPU Hours	22.2 CPU Hours	15.2 CPU Hours

* 64-bit variant of UNIX

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RADIATION-SHIELDING VALIDATION SUITE

Suite contains three categories of benchmarks

Time-of-flight spectra : Livermore pulsed spheres
Fusion shielding : ORNL D-T spectra
Photon dose rates : Skyshine, Air-over-ground, Hupmobile TLD

Cases include neutron-only, photon-only, and coupled neutron-photon calculations

All existing cases are taken from previous MCNP neutron and photon benchmark suites (LA-12212 and LA-12196)

Additional cases will be added in the near future

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CRITICALITY VALIDATION SUITE

Cases were selected to encompass a wide variety of

Fissile isotopes   : ^{233}U, ^{235}U, and ^{239}PU

Spectra   :   Fast, intermediate, and thermal

Compositions   :   Metals, oxides, and solutions

Configurations   :   Bare and reflected spheres and cylinders, 2-D and 3-D lattices, and infinite homogeneous and heterogeneous regions

^{235}U Cases were subdivided into HEU, IEU, AND LEU

Input specifications for all 31 cases are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

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CASES IN THE MCNP CRITICALITY VALIDATION SUITE

Spectrum	Fast			Intermed	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05	Falstaff-1*	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2	Flattop-25	Godiver	Zeus-2 UH$_3$	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H†	IEU-CT-02	STACY-36
LEU					B&W XI-2	LEU-ST-02
Pu	Jezebel Jezebel-240 Pu Buttons	Flattop-Pu THOR	Pu-MF-11	HISS/HPG†	PNL-33	PNL-2

* Extrapolated to critical
† k_∞ measurement

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PURPOSE AND USE OF THE
MCNP CRITICALITY VALIDATION SUITE

The MCNP Criticality Validation Suite was developed to assess the reactivity impact of future improvements to MCNP as well as changes to its associated nuclear data libraries

Suite is *not* an absolute indicator of the accuracy or reliability of a given nuclear data library, nor is it intended to be

Suite can provide a general indication of the overall performance of a nuclear data library

Suite can provide an early warning of unexpected or unintended consequences resulting from changes to nuclear data

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NUCLEAR DATA LIBRARIES FOR MCNP

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CONTINUOUS-ENERGY NUCLEAR DATA LIBRARIES

Library	Issued	Source	Identifiers	Total Nuclides	Nuclides with Probability Tables for Unresolved Resonance Region	Fissioning Nuclides with Delayed-Neutron Spectra
ENDF/B-V	1987	ENDF/B-V	.50c, .51c, .55c, .56c	~125	0	0
ENDF60	1994	ENDF/B-VI.2	.60c	122	0	0
ENDF66	2002	ENDF/B-VI.6	.64c, .65c, .66c	173	67	22
ACTI	2002	ENDF/B-VI.8	.61c, .62c, .63c	41	4	0

77° K   293° K   3000° K

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CONTINUOUS-ENERGY NUCLEAR DATA LIBRARIES
(Continued)

SAB2002, a library of thermal scattering laws $S(\alpha,\beta)$, was released in 2002

ACTI can be combined with ENDF66 to produce a nuclear data library that corresponds almost completely to the final release of ENDF/B-VI; that combination hereafter will be referred to as ENDF/B-VI

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MCNP5 CALCULATIONS
FOR CRITICALITY VALIDATION SUITE

Each calculation employed 550 generations with 10,000 neutrons per generation
(SB-5 and Zebra-8H employed 350 generations)

Results from first 50 generations were excluded from the statistics

Results therefore are based on 5,000,000 active histories for each case
(3,000,000 for SB-5 and Zebra-8H)

ENDF66 and ENDF/B-VI calculations used SAB2002

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RESULTS FOR ^{233}U BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI	ENDF66	ENDF60	ENDF/B-V
Jezebel-233	1.0000±0.0010	0.9931±0.0002	0.9931±0.0002	0.9928±0.0003	0.9930±0.0003
Flattop-23	1.0000±0.0014	1.0003±0.0003	1.0003±0.0003	1.0008±0.0003	1.0016±0.0003
U233-MF-05	1.0000±0.0030	0.9976±0.0003	0.9963±0.0005	0.9971±0.0003	0.9968±0.0003
Falstaff-1	1.0000±0.0083	0.9894±0.0005	0.9902±0.0005	0.9890±0.0005	0.9864±0.0005
SB-2½	1.0000±0.0024	0.9967±0.0005	0.9974±0.0005	0.9978±0.0005	1.0007±0.0005
ORNL-11	1.0006±0.0029	0.9968±0.0002	0.9974±0.0002	0.9956±0.0002	0.9987±0.0002

$1\sigma < \Delta k \leq 2\sigma$ $\Delta k > 2\sigma$

ENDF/B-VI results for thermal cases are significantly lower than ENDF/B-V results

Other reactivity changes are fairly small (final ^{233}U cross sections are unchanged from ENDF/B-VI.0)

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RESULTS FOR HEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI	ENDF66	ENDF60	ENDF/B-V
Godiva	1.0000±0.0010	0.9962±0.0003	0.9962±0.0003	0.9965±0.0003	0.9979±0.0003
Tinkertoy-2	1.0000±0.0038	0.9972±0.0003	0.9972±0.0003	0.9987±0.0003	0.9983±0.0003
Flattop-25	1.0000±0.0030	1.0024±0.0003	1.0024±0.0005	1.0027±0.0003	1.0036±0.0003
Godiver	0.9985±0.0011	0.9948±0.0003	0.9954±0.0004	0.9970±0.0003	0.9968±0.0003
UH$_3$	1.0000±0.0047	0.9914±0.0003	0.9915±0.0003	1.0080±0.0004	0.9943±0.0003
Zeus-2	0.9997±0.0008	0.9942±0.0003	0.9941±0.0003	1.0088±0.0004	0.9992±0.0004
SB-5	1.0015±0.0028	0.9963±0.0005	0.9980±0.0005	0.9972±0.0005	0.9963±0.0006
ORNL-10	1.0015±0.0026	0.9992±0.0002	0.9990±0.0002	0.9970±0.0002	1.0000±0.0002

ENDF/B-V produces best overall results for fast and intermediate cases

ENDF66 produces best results for thermal cases

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RESULTS FOR IEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI	ENDF66	ENDF60	ENDF/B-V
IEU-MF-03	1.0000±0.0017	0.9987±0.0003	0.9989±0.0003	1.0001±0.0003	1.0053±0.0003
BIG TEN	0.9948±0.0013	1.0071±0.0003	1.0071±0.0003	1.0043±0.0002	1.0043±0.0002
IEU-MF-04	1.0000±0.0030	1.0038±0.0003	1.0038±0.0003	1.0044±0.0003	1.0088±0.0003
Zebra-8H	1.0300±0.0025	1.0405±0.0002	1.0407±0.0002	1.0304±0.0002	1.0202±0.0002
IEU-CT-02	1.0017±0.0044	1.0007±0.0003	1.0003±0.0003	1.0010±0.0003	1.0023±0.0003
STACY-36	0.9988±0.0013	0.9988±0.0003	0.9985±0.0003	0.9964±0.0003	1.0002±0.0003

Introduction of probability-table treatment for unresolved resonance region substantially increases reactivity for BIG TEN and especially Zebra-8H

Reversion to ENDF/B-V value for 1/v capture in H, introduced in ENDF/B-VI.5, is primarily responsible for improvement in k_{eff} for STACY-36

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RESULTS FOR LEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI	ENDF66	ENDF60	ENDF/B-V
B&W XI-2	1.0007±0.0012	0.9968±0.0003	0.9968±0.0003	0.9965±0.0003	0.9984±0.0003
LEU-ST-02	1.0024±0.0037	0.9957±0.0003	0.9955±0.0003	0.9916±0.0003	0.9964±0.0003

Reversion to ENDF/B-V value for 1/v capture in H, introduced in ENDF/B-VI.5, is primarily responsible for improvement in k_{eff} for LEU-ST-02

ENDF/B-V produces best overall results for these cases

ENDF66 produces worst overall results for these cases

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RESULTS FOR PU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VI	ENDF66	ENDF60	ENDF/B-V
Jezebel	1.0000±0.0020	0.9975±0.0003	0.9975±0.0003	0.9974±0.0003	0.9977±0.0003
Jezebel-240	1.0000±0.0020	0.9979±0.0003	0.9979±0.0003	0.9985±0.0003	0.9987±0.0003
Pu Buttons	1.0000±0.0030	0.9962±0.0003	0.9963±0.0003	0.9969±0.0003	0.9959±0.0003
Flattop-Pu	1.0000±0.0030	1.0019±0.0003	1.0019±0.0004	1.0032±0.0003	1.0026±0.0003
THOR	1.0000±0.0006	1.0062±0.0003	1.0062±0.0003	1.0062±0.0003	1.0049±0.0003
Pu-MF-11	1.0000±0.0010	0.9970±0.0003	0.9969±0.0003	0.9980±0.0004	1.0007±0.0004
HISS/HPG	1.0000±0.0110	1.0105±0.0003	1.0105±0.0002	1.0105±0.0002	1.0075±0.0002
PNL-33	1.0024±0.0021	1.0029±0.0003	1.0036±0.0003	1.0015±0.0003	1.0077±0.0003
PNL-2	1.0000±0.0065	1.0033±0.0005	1.0036±0.0005	1.0006±0.0005	1.0081±0.0004

Results from ENDF/B-VI libraries show improvement for thermal cases relative to ENDF/B-V, but k_{eff} for water-reflected Pu sphere gets progressively worse

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SUMMARY OF RESULTS FOR
MCNP CRITICALITY VALIDATION SUITE

Range	ENDF/B-VI	END66	ENDF60	ENDF/B-V
$|\Delta k| \leq \sigma$	13	12	13	11
$\sigma < |\Delta k| \leq 2\sigma$	9	10	12	13
$|\Delta k| > 2\sigma$	9	9	6	7

Overall, ENDF60 produces best results, although not dramatically so

ENDF60 underpredicts reactivity for thermal uranium cases (especially LEU) and overpredicts it for HEU cases with intermediate spectra

Relative to ENDF/B-V, ENDF/B-VI shows improved results for fast IEU and thermal plutonium systems but worse results for thermal [233]U systems, intermediate HEU systems, and B&W XI-2

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FORTHCOMING IMPROVEMENTS IN NUCLEAR DATA

MCNP Workshop
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April 25, 2004

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PRE-ENDF/B-VII

Are future nuclear data libraries likely to produce improved results?

Preliminary changes to ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu for ENDF/B-VII offer encouragement

Data changes primarily involve high-energy elastic and inelastic scattering in the uranium isotopes and ^{239}Pu (LANL group T-16), as well as resonance parameters for ^{238}U (ORNL)

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RESULTS FOR ^{233}U BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VII	ENDF/B-VI
Jezebel-233	1.0000±0.0010	0.9984±0.0003	0.9931±0.0003
Flattop-23	1.0000±0.0014	0.9988±0.0003	1.0003±0.0003
U233-MF-05	1.0000±0.0030	0.9964±0.0003	0.9976±0.0003
Falstaff-1	1.0000±0.0083	0.9876±0.0005	0.9894±0.0005
SB-2½	1.0000±0.0024	0.9946±0.0005	0.9967±0.0005
ORNL-11	1.0006±0.0029	1.0002±0.0002	0.9968±0.0002

k_{eff} for Jezebel-233 improves dramatically, and reactivity swing from Jezebel-233 to Flattop-23 is eliminated

k_{eff} for ORNL-10 improves substantially, although result for SB-2½ deteriorates

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RESULTS FOR HEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VII	ENDF/B-VI
Godiva	1.0000±0.0010	0.9992±0.0003	0.9962±0.0003
Tinkertoy-2	1.0000±0.0038	1.0001±0.0003	0.9972±0.0003
Flattop-25	1.0000±0.0030	1.0025±0.0003	1.0024±0.0003
Godiver	0.9985±0.0011	0.9978±0.0004	0.9948±0.0003
UH_3	1.0000±0.0047	0.9926±0.0003	0.9914±0.0003
Zeus-2	0.9997±0.0008	0.9948±0.0003	0.9942±0.0003
SB-5	1.0015±0.0028	0.9943±0.0005	0.9963±0.0005
ORNL-10	1.0015±0.0026	0.9994±0.0002	0.9992±0.0002

k_{eff} improves substantially for Godiva and Godiver but deteriorates for SB-5

Reactivity swing from Godiva to Flattop-25 is reduced significantly

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RESULTS FOR IEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VII	ENDF/B-VI
IEU-MF-03	1.0000±0.0017	1.0026±0.0003	0.9987±0.0003
BIG TEN	0.9948±0.0013	0.9950±0.0003	1.0071±0.0002
IEU-MF-04	1.0000±0.0030	1.0077±0.0003	1.0038±0.0003
Zebra-8H	1.0300±0.0025	1.0190±0.0002	1.0405±0.0002
IEU-CT-02	1.0017±0.0044	1.0005±0.0003	1.0007±0.0003
STACY-36	0.9988±0.0013	0.9983±0.0003	0.9988±0.0003

k_{eff} improves dramatically for BIG TEN

k_{eff} is worse for IEU-MF-03 and IEU-MF-04

k_{eff} drops substantially for Zebra-8H

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RESULTS FOR LEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VII	ENDF/B-VI
B&W XI-2	1.0007±0.0012	0.9997±0.0003	0.9968±0.0003
LEU-ST-02	1.0024±0.0037	0.9957±0.0003	0.9957±0.0003

k_{eff} improves substantially for B&W XI-2 (much better than from ENDF/B-VI)

Eliminates need for *ad hoc* adjustment to ^{238}U resonance integral (used in many data libraries since early 1970s)

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RESULTS FOR PU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}	
		ENDF/B-VII	ENDF/B-VI
Jezebel	1.0000±0.0020	1.0004±0.0003	0.9975±0.0003
Jezebel-240	1.0000±0.0020	1.0001±0.0003	0.9979±0.0003
Pu Buttons	1.0000±0.0030	0.9986±0.0003	0.9962±0.0003
Flattop-Pu	1.0000±0.0030	1.0006±0.0003	1.0019±0.0003
THOR	1.0000±0.0006	1.0081±0.0003	1.0062±0.0003
Pu-MF-11	1.0000±0.0010	0.9986±0.0003	0.9970±0.0003
HISS/HPG	1.0000±0.0110	1.0111±0.0003	1.0105±0.0003
PNL-33	1.0024±0.0021	1.0057±0.0003	1.0029±0.0003
PNL-2	1.0000±0.0065	1.00390.0005	1.0033±0.0005

Striking improvement in k_{eff} for fast cases except THOR, and reactivity swing from Jezebel to Flattop-Pu is eliminated

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SUMMARY OF RESULTS FOR
MCNP CRITICALITY VALIDATION SUITE

Range	Pre-ENDF/B-VII	ENDF/B-VI
$|\Delta k| \leq \sigma$	17	13
$\sigma < |\Delta k| \leq 2\sigma$	8	9
$|\Delta k| > 2\sigma$	6	9

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CONCLUSIONS

Overall, Pre-ENDF/B-VII produces major reactivity improvements relative to ENDF/B-VI

Reactivity swings from bare spheres to similar systems reflected by normal uranium are eliminated or substantially reduced

Need for *ad hoc* adjustment to ^{238}U resonance integral may be eliminated

Improvements still are needed, particularly for cases with intermediate spectra or with thorium

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TEMPERATURE-SPECIFIC NUCLEAR DATA LIBRARIES

AND THE DOPPLER CODE

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BACKGROUND

MCNP requires nuclear data at the temperature of interest

Most existing nuclear data libraries for MCNP contain cross sections for a very limited number of temperatures (e.g., 77° K, 293.6° K, 3000° K in ENDF66 and ACTI)

This requirement constitutes an obstacle for many reactor-physics calculations, most of which are performed at a variety of elevated temperatures

In principle, cross sections at a given temperature could be adjusted to the temperature of interest using the same procedures employed to generate the initial nuclear data library

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DOPPLER

DOPPLER was written by Bob MacFarlane (LANL group T-16), the principal author of NJOY

DOPPLER broadens resonance cross sections using the same kernel-broadening method as NJOY

DOPPLER uses a fixed fitting tolerance of 0.1% and default thinning options from NJOY

For thermal scattering laws ($S(\alpha,\beta)$), DOPPLER interpolates between two sets of data that bracket the temperature of interest

For probability tables for the unresolved resonance range, DOPPLER again interpolates between two sets of data that bracket the temperature of interest

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LIBRARY COMPATIBILITY

DOPPLER is fully compatible with ACTI, ENDF66, and SAB2002

Problems may or may not arise if DOPPLER is applied to earlier MCNP data libraries or libraries generated outside of LANL,depending upon the specifics of how they were generated and the nuclides of interest

IRPhEP HOT KRITZ:2 BENCHMARKS

Core	Fuel Type	Array Size	Cold Fuel Radius (cm)	Cold Pitch (cm)	Temp (°C)	Soluble Boron (ppm)	Water Height (cm)	Axial Buckling (10^{-4} cm^{-2})
Kritz:2-1	UO$_2$ 1.86 w/o	44x44	0.529	1.485	248.5	26.2	105.52	6.25
Kritz:2-13	UO$_2$ 1.86 w/o	40x40	0.529	1.635	243.0	280.1	110.96	5.98
Kritz-2:19	MOX 1.50 w/o	25x24	0.5395	1.800	235.9	5.2	100.01	7.70

These benchmarks appeared to be ideal candidates to test the adequacy of DOPPLER

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KRITZ 2-D BENCHMARK

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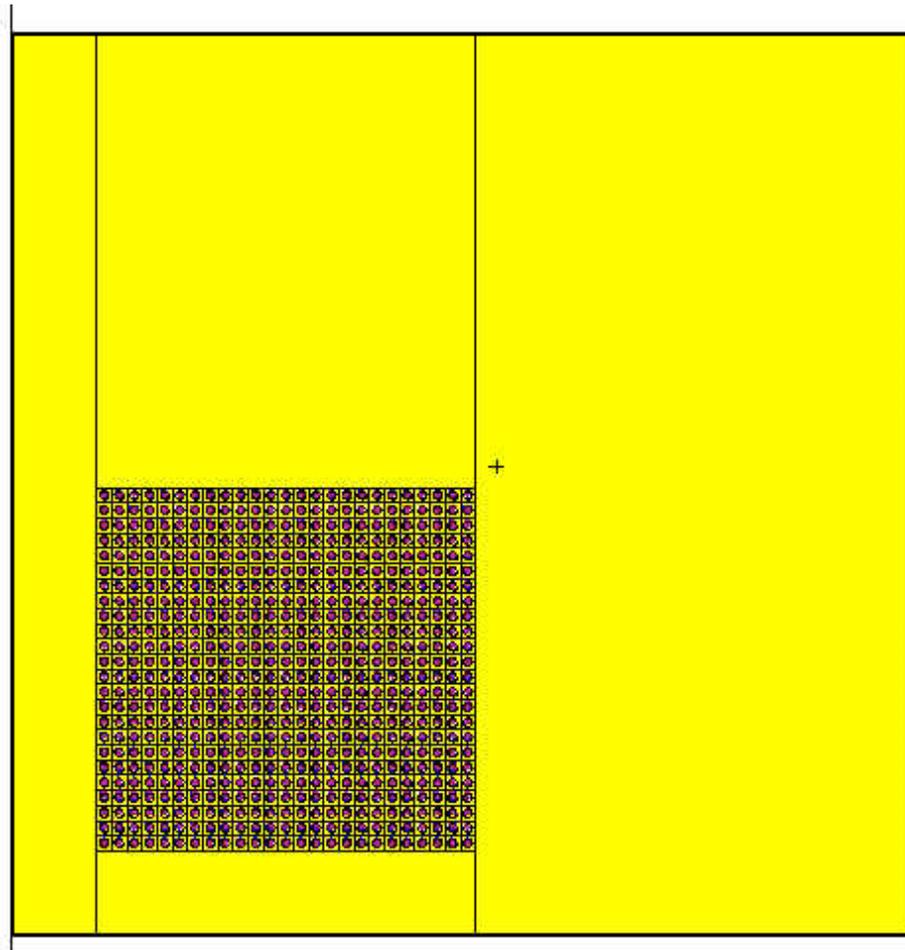
NUCLEAR DATA FOR HOT BENCHMARKS

Separate nuclear data sets were generated at 245 °C using DOPPLER and NJOY (generated and tested by Bob Little, LANL group X-5)

Basic data were taken from ENDF/B-VI Release 6 (same as ENDF66)

MCNP5 calculations were performed for the hot 2-D benchmarks, and the results from the two data sets were compared

Each calculation employed 550 generations with 10,000 neutron histories per generation

Results from first 50 generations were discarded $\Rightarrow$ 5,000,000 active histories for each case

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MCNP5 RESULTS FROM DOPPLER AND NJOY LIBRARIES

Case	Library	k_{eff}	Δk
Kritz:2-1	NJOY	0.9914 ± 0.0003	—
	DOPPLER	0.9911 ± 0.0003	-0.0003 ± 0.0004
Kritz:2-13	NJOY	0.9944 ± 0.0003	—
	DOPPLER	0.9942 ± 0.0003	-0.0002 ± 0.0004
Kritz:2-19	NJOY	1.0005 ± 0.0003	—
	DOPPLER	1.0009 ± 0.0003	0.0004 ± 0.0004

Conclusion: DOPPLER produces nuclear data that are consistent with those generated directly with NJOY

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DOPPLER INPUT FILE

path=(location of initial data file)
```
1001.66c    0 4.386e-8   1001.01c
5010.66c    0 4.386e-8   5010.01c
5011.66c    0 4.386e-8   5011.01c
8016.66c    0 4.386e-8   8016.01c
8017.66c    0 4.386e-8   8017.01c
24050.66c  0 4.386e-8   24050.01c
24052.66c  0 4.386e-8   24052.01c
24053.66c  0 4.386e-8   24053.01c
24054.66c  0 4.386e-8   24054.01c
26054.66c  0 4.386e-8   26054.01c
26056.66c  0 4.386e-8   26056.01c
26057.66c  0 4.386e-8   26057.01c
26058.66c  0 4.386e-8   26058.01c
28058.66c  0 4.386e-8   28058.01c
28060.66c  0 4.386e-8   28060.01c
```

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DOPPLER INPUT FILE (CONT'D)

```
28061.66c  0 4.386e-8   28061.01c
28062.66c  0 4.386e-8   28062.01c
28064.66c  0 4.386e-8   28064.01c
40000.66c  0 4.386e-8   40000.01c
92235.66c  92235.65c  4.386e-8   92235.01c
92238.66c  92238.65c  4.386e-8   92238.01c
94239.66c  94239.65c  4.386e-8   94239.01c
94240.66c  94240.65c  4.386e-8   94240.01c
94241.66c  94241.65c  4.386e-8   94241.01c
94242.66c  94242.65c  4.386e-8   94242.01c
95241.66c  95241.65c  4.386e-8   95241.01c
lwtr.61t   lwtr.62t   4.386e-8   lwtr.01t
end
```

CURRENT STATUS OF DOPPLER

DOPPLER currently is undergoing final technical review

Draft version of users' manual has been written and reviewed

Additional review will be required prior to distribution

For more information, contact:

> Dr. Robert E. MacFarlane
> Los Alamos National Laboratory
> ryxm@lanl.gov

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REMINDER

MCNP users who have not yet upgraded to MCNP5 should be aware of the following notice, which appears in the April 2004 edition of the RSICC Newsletter. The request form may be accessed at http//www-rsicc.ornl.gov/rsiccnew/order.htm.

MCNP5 Notice

April is the final month that the user fee for the MCNP5 package will be waived for requesters who received a prior version of MCNP from RSICC. Complete a request form and select the MCNP5 (C00710MNYCP01) package. In the comments field, please state your name and the installation at which you received the earlier version for verification.

MCNP Workshop
PHYSOR 2004
April 25, 2004

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**Diagnostics
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Improvements & Enhancements

-

Work in Progress

- **Proton transport**
  - Continuous-energy physics up to 50 GeV
  - Direct tracking through magnetic fields
  - COSY-map tracking through magnetic fields
- **Many additional particle types**

- **ENDF/B-VII** (Data Team)
- **Improved electron transport**
- **Automated variance reduction, using deterministic adjoint**
- **Isotopic source**
- **Criticality**
  - Source convergence diagnostics (relative entropy)
  - Dominance ratio
  - Perturbation theory – corrections for changing source shape in criticality
  - Fission neutron multiplicity
  - Fission matrix
- **Continuously varying material properties & tallies**
- Etc.

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Monte Carlo Eigenvalue Calculations & Theory

Taro Ueki (UNM)

Forrest Brown, Russ Mosteller

K-Calculations -- Convergence
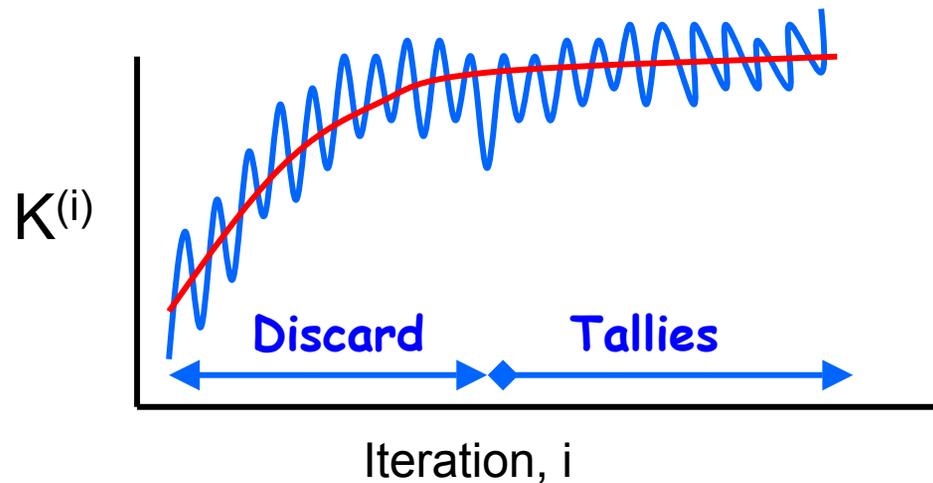
Monte Carlo

Deterministic (Sn)

$K^{(i)}$

Discard   Tallies

Iteration, i

- Guess an initial source distribution

- Iterate until converged   (How do you know ???)

- Then

  – For Sn code: done, print the results

  – For Monte Carlo: start tallies, keep running until uncertainties small enough

- **Batch size? Convergence? Stationarity? Bias? Statistics?**

- **Some number of initial cycles must be discarded**

  – The source distribution & Keff are not known initially

  – Guess at the source & Keff

  – Iterate, discarding tallies

  – When converged, iterate to accumulate tallies

- Number of iterations to discard depends on the **dominance ratio**

  – **Dominance Ratio = K_1 / K_{eff}**

    • K_{eff} = eigenvalue of fundamental eigenmode

    • K_1 = eigenvalue of first higher eigenmode, $K_1 < K_{eff}$

  – If DR close to 1 (eg, .999…), 100s or 1000s of initial iterations may be required for initial source distribution errors to die away

  – Most statistical tests for convergence are *ex post facto* tests to look for trends

  – Most common practice is to examine plots of Keff vs cycles

- **K-effective calculations**

$$\Psi^{(n+1)} = R \bullet \Psi^{(n+1)} + \frac{1}{K_{eff}^{(n)}} F \bullet \Psi^{(n)}$$

$$\Psi^{(n+1)} = \frac{1}{K_{eff}^{(n)}} [I - R]^{-1} F \bullet \Psi^{(n)} \qquad\qquad K_{eff}^{(n)} = \int F \bullet \Psi^{(n)} dp dp'$$

Where $\Psi^{(n)}$ = neutron source points from fission in n-th cycle

= k-effective estimate from n-th cycle

F   = fission kernel

Monte Carlo process:

Simulate neutron from birth at r', through history,

to production of next-generation neutron from fission at r.
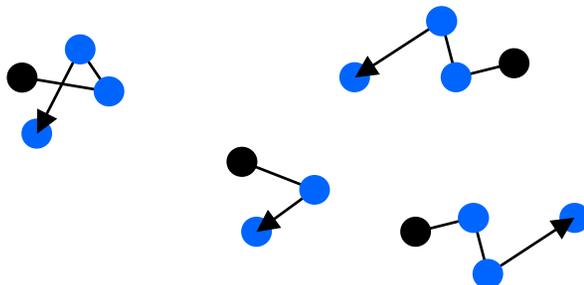
● **Neutron source site from cycle n**

● **Neutron source site for cycle n+1**

Correlation & Criticality Calculations

- Correlation
  - Spatial locations of fission sites in cycle **n** are **correlated** to the site locations in previous cycles.
  - Cycle-to-cycle correlation effects can be significant for:
    - Large reactors, with small leakage
    - Heavy-water moderated or reflected reactors
    - Loosely-coupled systems
- Computed variances are usually **nonconservative** (too small), due to cycle-to-cycle correlation

- CHALLENGE: Compute variances correctly, even when correlation is significant

- OPPORTUNITY: Theory & model for correlation effects, use this for new types of computations

Convergence, Correlation, Dominance Ratio

Initial guess

Exact solution
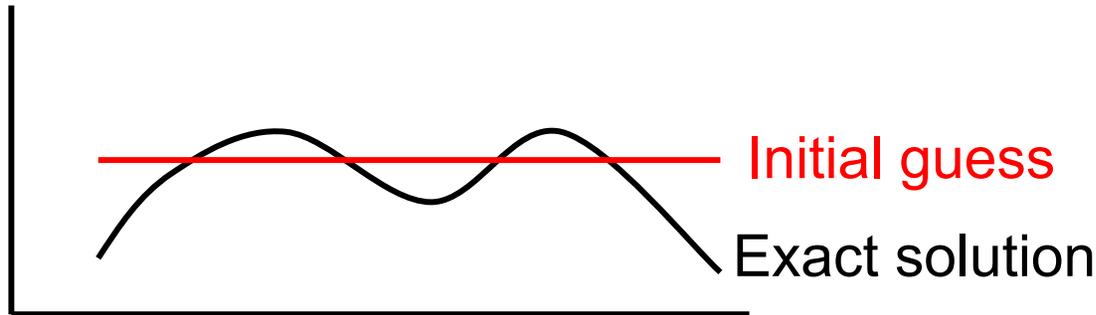
- For inverse power iteration:

  – Error in initial guess dies off as $\sim (DR)^n$

  – To reduce 10% error $\rightarrow$ .1% error

      DR~.9 $\rightarrow$ 44 iterations
      DR~.99 $\rightarrow$ 458 iterations
      DR~.999 $\rightarrow$ 2301 iterations

Noise (fluctuation)

Exact solution
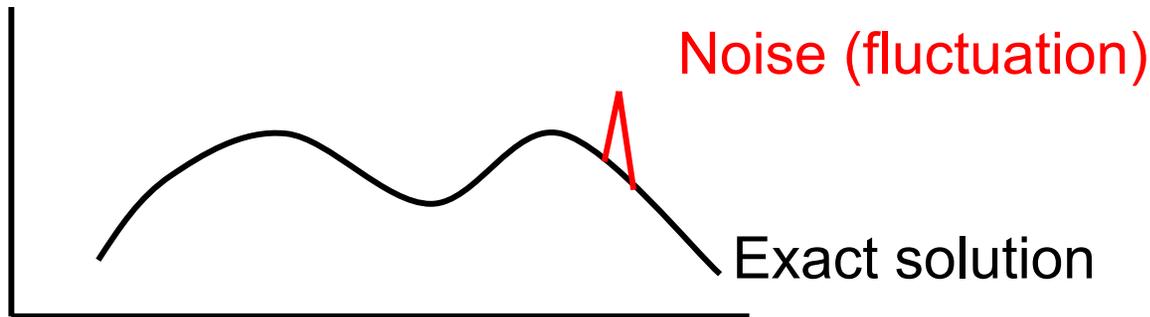
- **For Monte Carlo power iteration,**

  statistical fluctuations in source shape die out gradually over a number of successive iterations.

  - Persistance of the noise over successive iterations gives correlation among source distributions in successive iterations. (<u>Positive</u> correlation)

  - Correlation directly affects confidence intervals:

    Serial correlation in source distribution ➔ larger confidence intervals

- **Most Monte Carlo codes ignore these correlation effects & incorrectly <u>underestimate</u> the confidence intervals**

In a series of related papers, we have significantly extended the theory of Monte Carlo eigenvalue calculations, explicitly accounting for correlation effects.   (see MCNP website: `www-xdiv.lanl.gov/x5/MCNP`)

LA-UR-02-0190:   T Ueki, **"Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations"**, Nucl. Sci. Eng. (2002)

LA-UR-01-6770:   T Ueki & FB Brown, "**Autoregressive Fitting for Monte Carlo K-effective Confidence Intervals**", Trans ANS (June 2002)

LA-UR-02-3783:   T Ueki & FB Brown, "**Stationarity Diagnostics Using Shannon Entropy in Monte Carlo Criticality Calculations I: F Test**",
Trans ANS (Nov 2002)

LA-UR-02-6228:   T Ueki & FB Brown, "**Stationarity and Source Convergence in Monte Carlo Criticality Calculations**", ANS M&C Topical Meeting (April, 2003)

LA-UR-03-0106:   T Ueki, FB Brown, DK Parsons, "**Dominance Ratio Computation via Time Series Analysis of Monte Carlo Fission Sources**" , Trans ANS (June 2003)

LA-UR-02-5700:   T Ueki, FB Brown, DK Parsons, & DE Kornreich, "**Autocorrelation and Dominance Ratio in Monte Carlo Criticality Calculations**",
Nucl. Sci. Eng. (Nov, 2003)

LA-UR-03-5823:   T Ueki, FB Brown, DK Parsons, JS Warsa, "**Time Series Analysis of Monte Carlo Fission Sources: I. Dominance Ratio Calculation**", Nucl. Sci. Eng.
(Nov. 2004)

LA-UR-03-????:   T Ueki & FB Brown, "**Stationarity Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations**,"
submitted to Nucl. Sci. Eng.

- Keff is an integral quantity - converges faster than source shape

Keff calculation for 2 nearly symmetric slabs, with Dominance Ratio = .9925
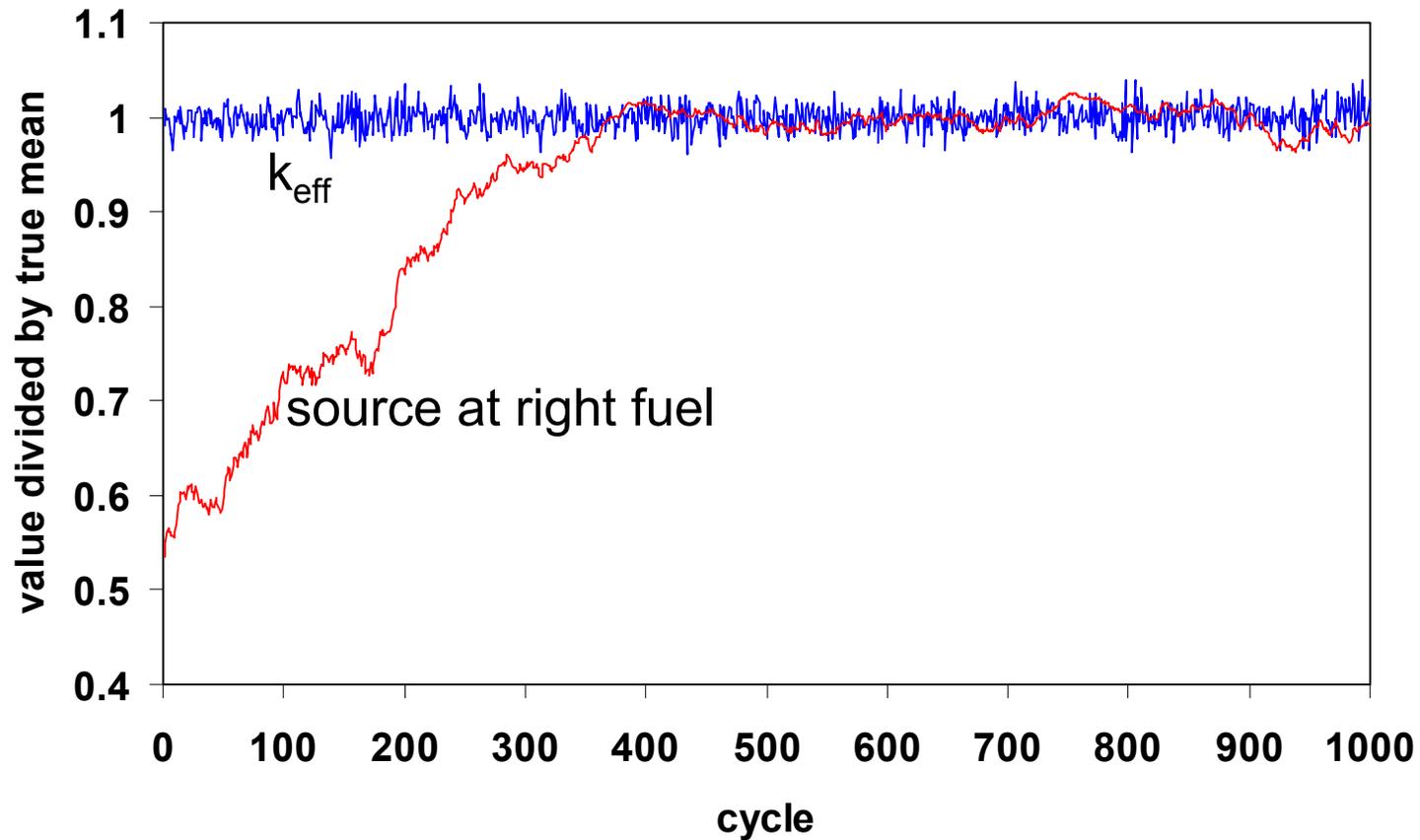
• Shannon entropy of the source distribution tallies has been found to be a good measure of convergence & stationarity

• Relative entropy is used in practice
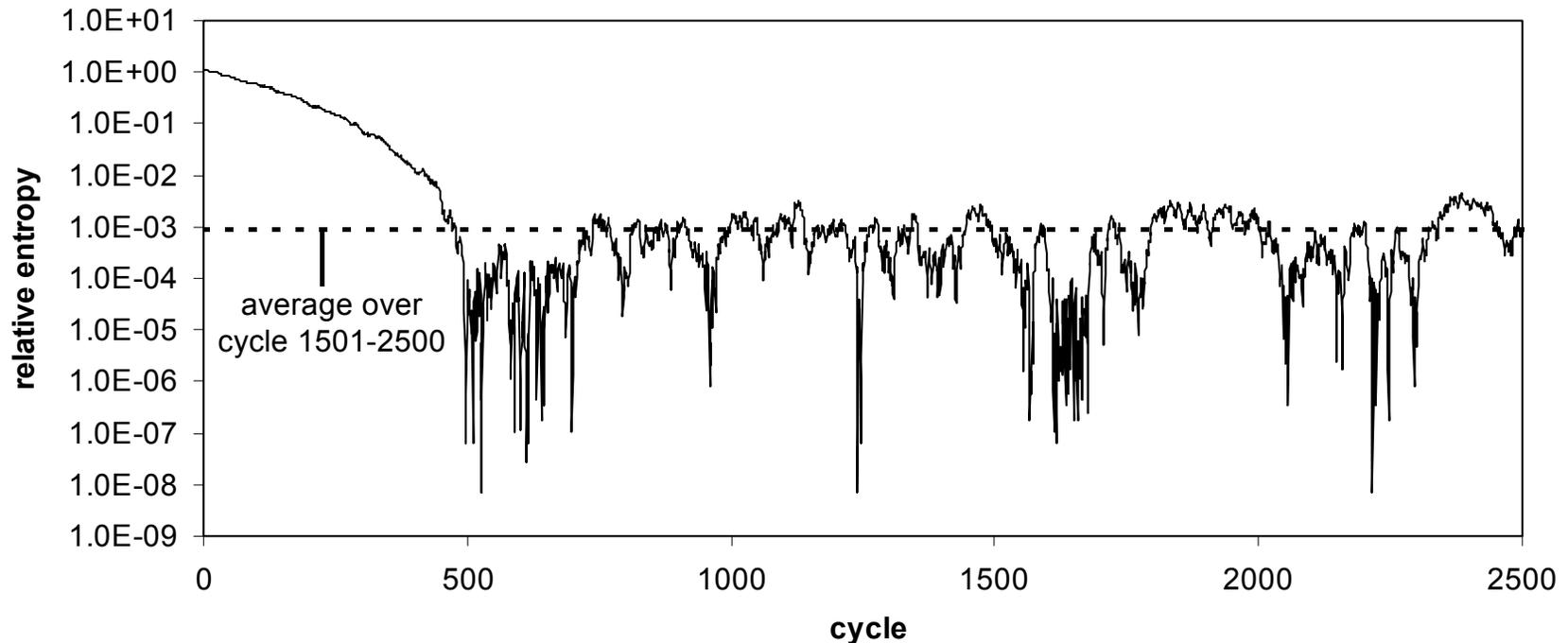
Figure 3: Posterior computation of relative entropy assuming the true source is the mean source over 1501-2500 cycles (problem 1)

Stationarity Tests

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- Plots of single-cycle Keff or cumulative Keff are difficult to interpret when assessing convergence

Cycle k$_{eff}$

50000 histories per cycle

— uniform initial source
— initial source at (1,3) lattice
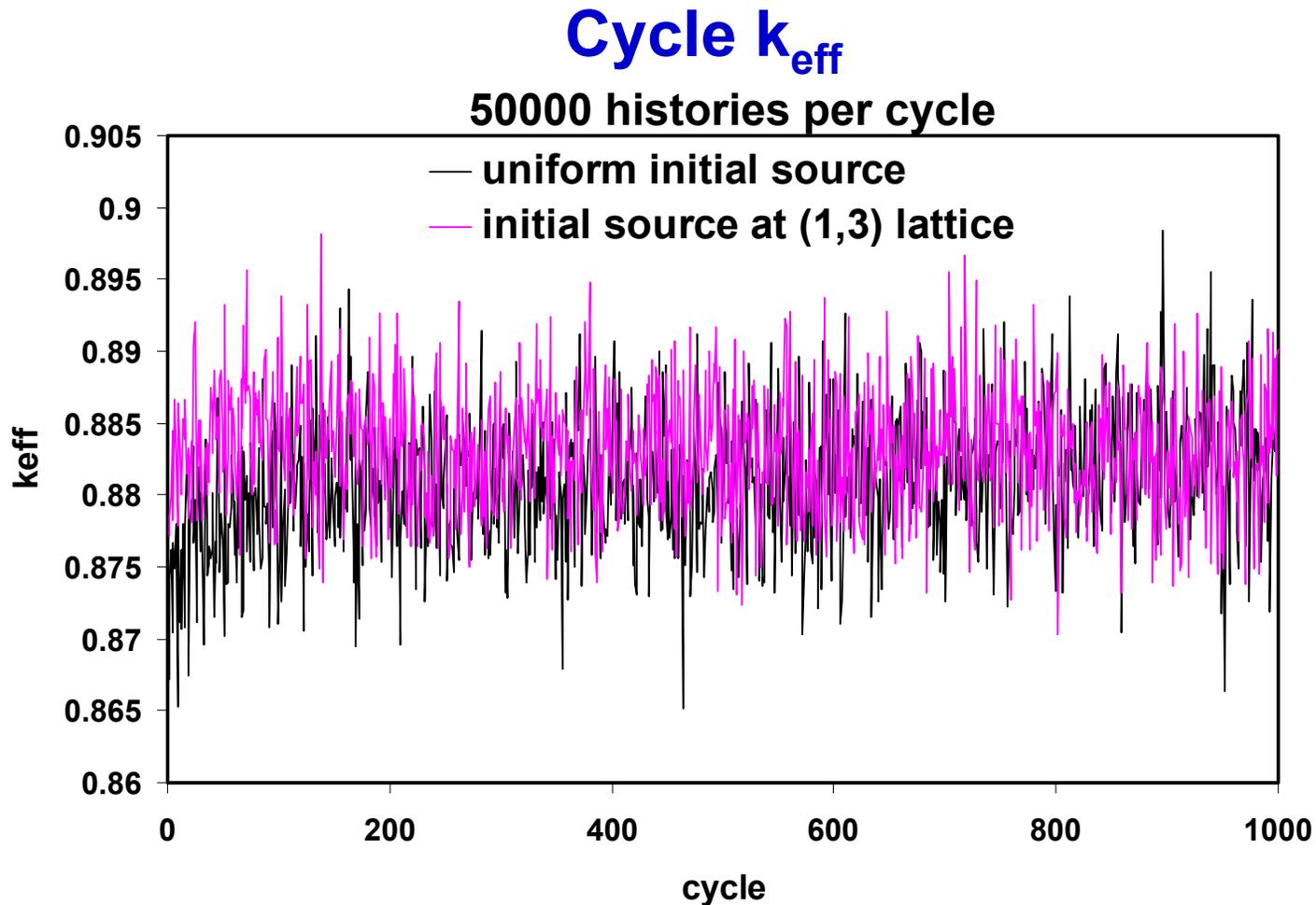
Posterior relative entropy
(500 inactive and 500 active cycles)

Stationarity Tests

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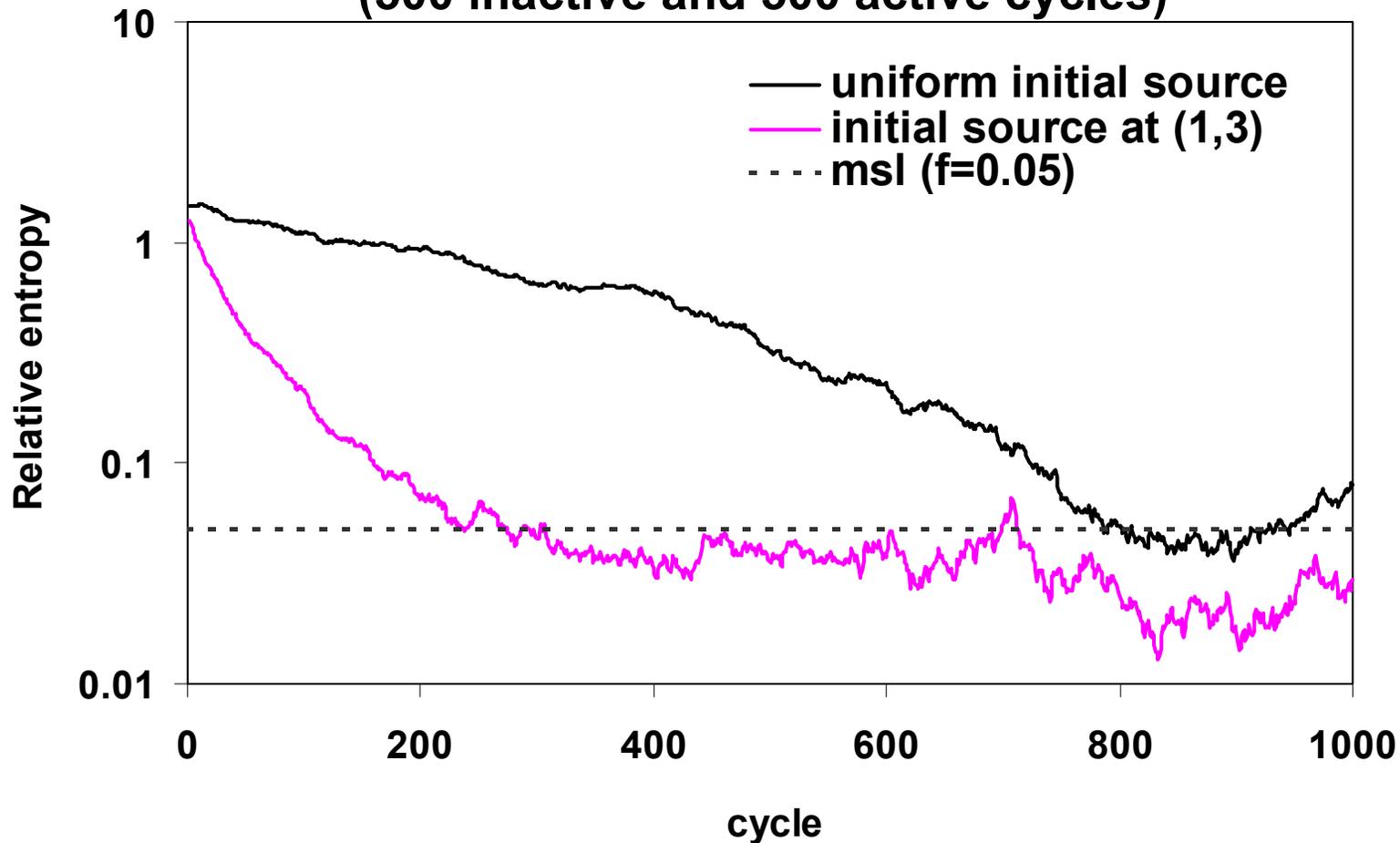
- The MCNP team has been investigating new stationarity tests

Progressive relative entropy
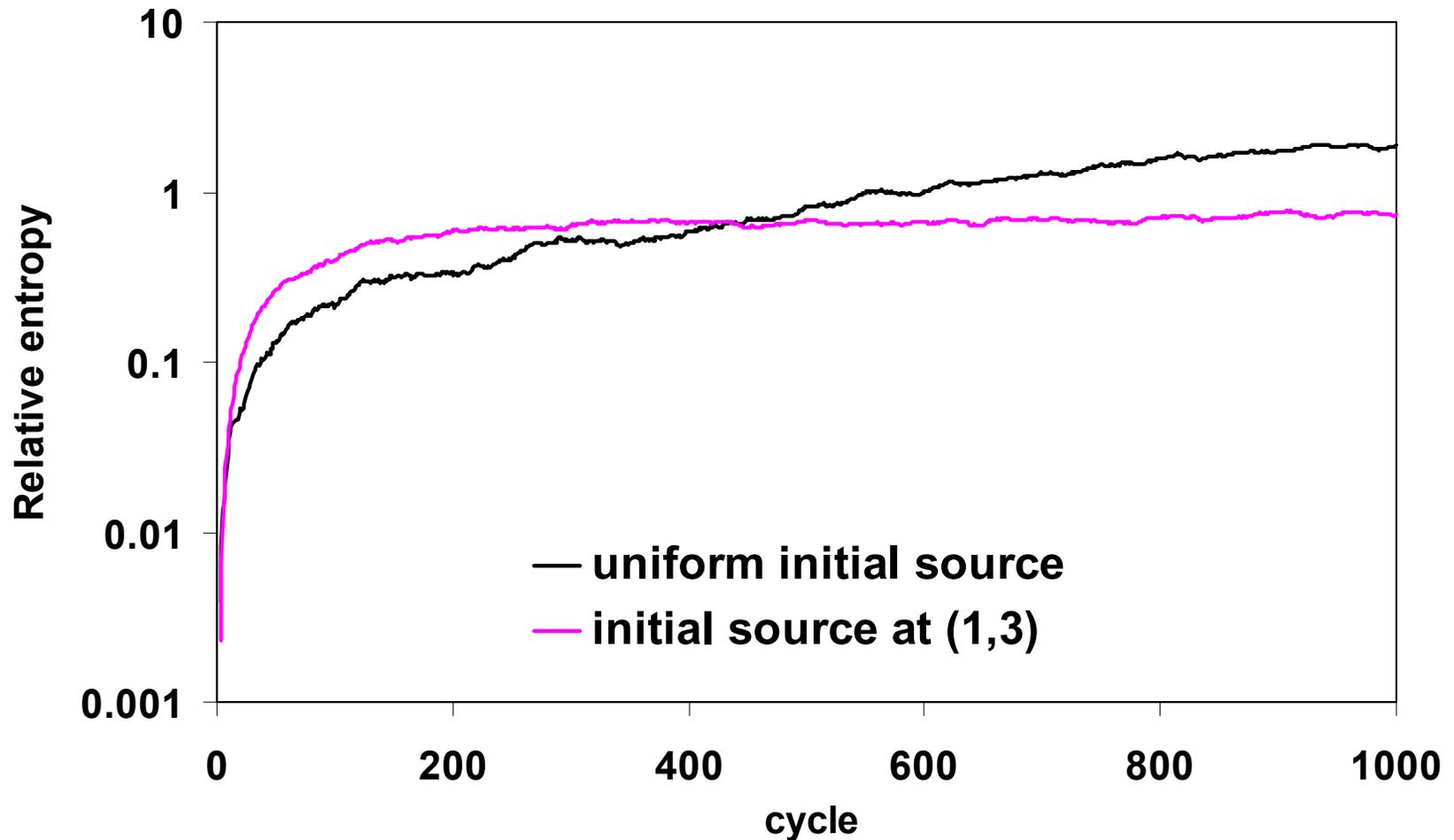
One cycle delay embedding plot of relative entropy wrt initial source
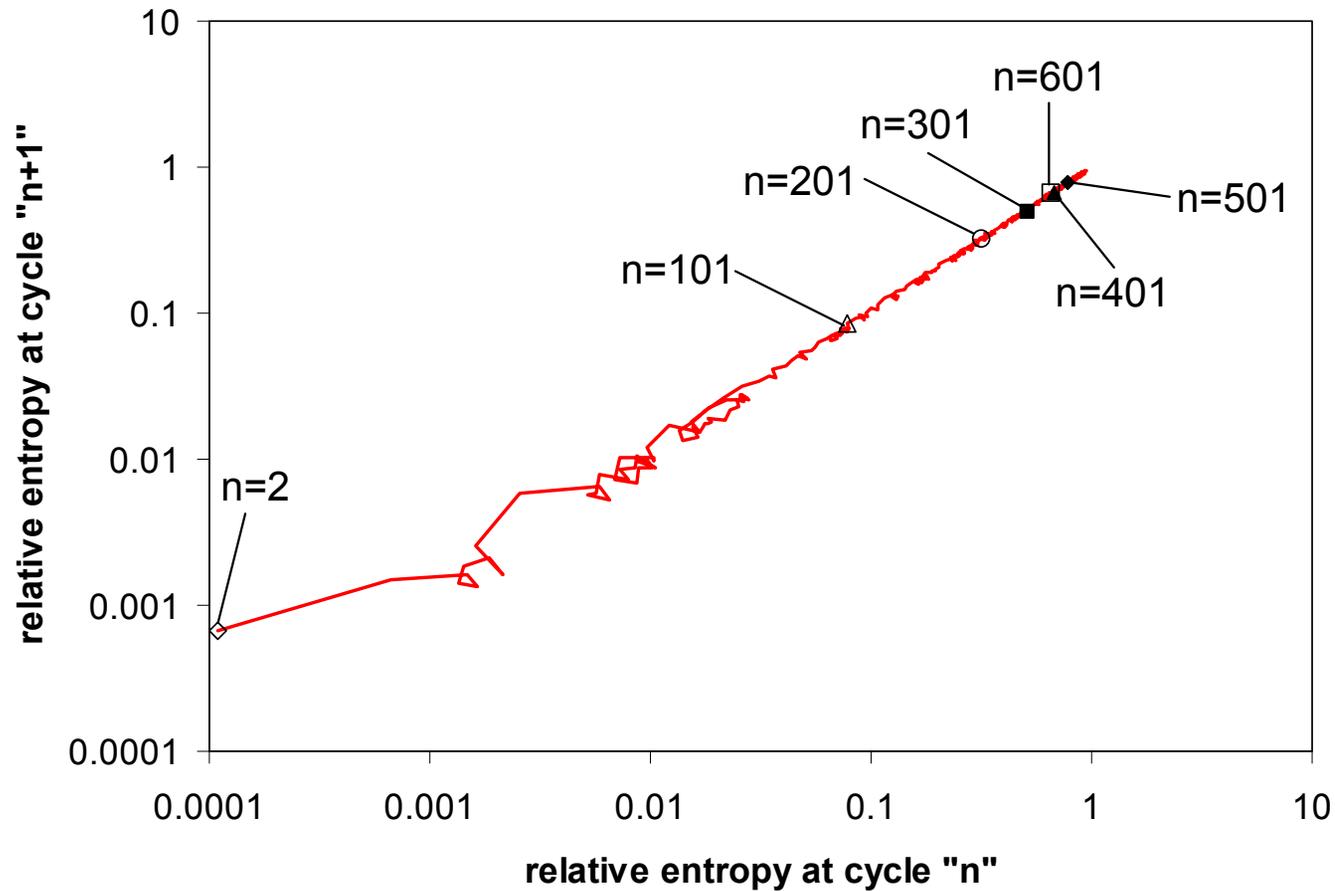
- After the source distribution is stationary, time series analysis can produce the dominance ratio (K_1/K_{eff})

- This is the first known successful technique for calculating the dominance ratio with a continuous Monte Carlo code

  Note:

  – MC codes which produce a fission matrix could compute the dominance ratio for the fission matrix. This would approach the dominance ratio of the physical problem as the fission matrix mesh is refined. Usually, computer storage limits prevent such refinement.

  – The present method is not dependent on a mesh, & can yield accurate results for any problem

  – See LA-UR-03-5823 & LA-UR-02-5700 on the MCNP website

Dominance ratio of 2D homogeneous square problems (95% (1.96σ) CI)
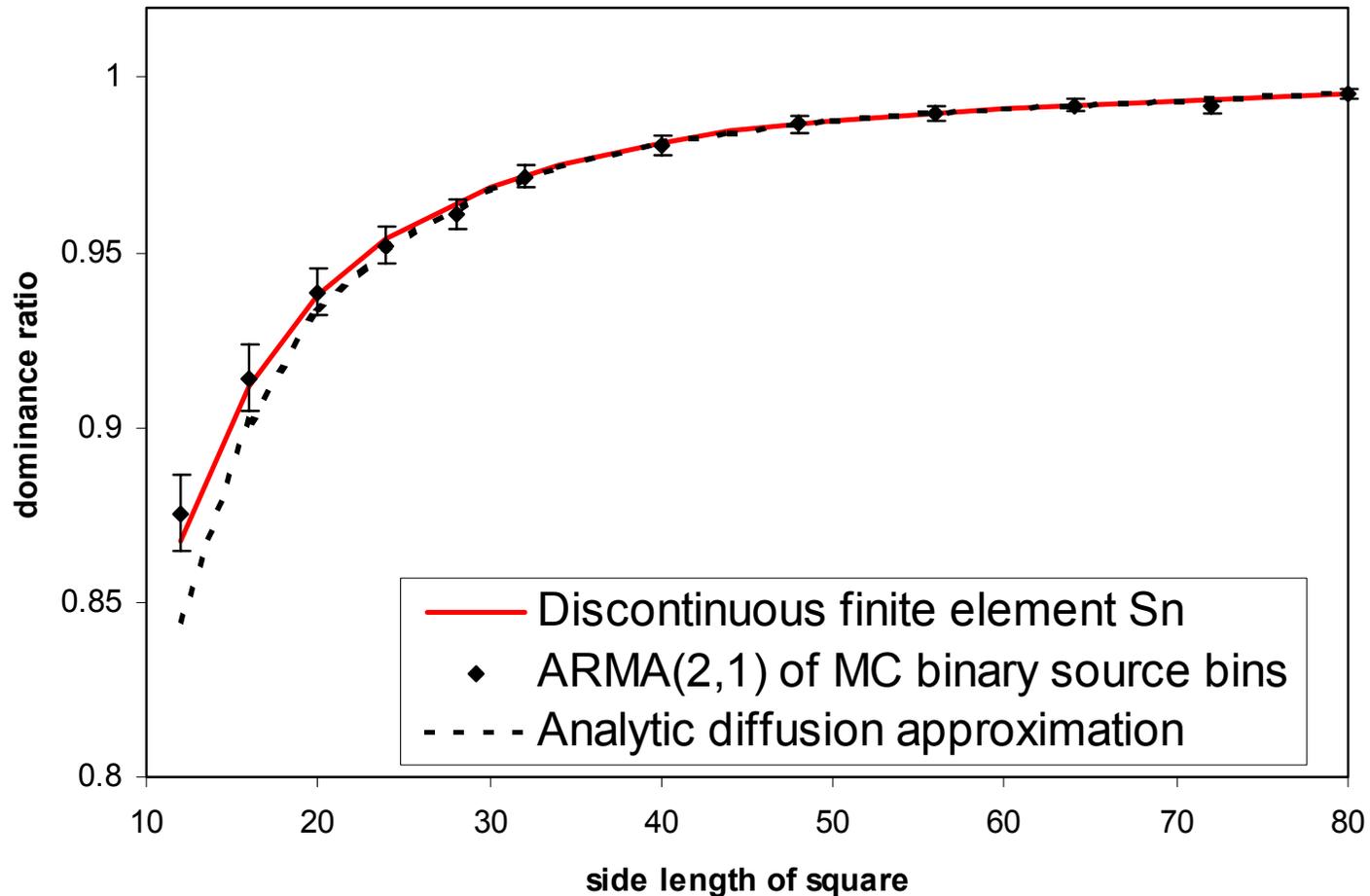
Perturbation Theory Improvements

Yasunobu Nagaya (JAERI),

Forrest Brown, Russ Mosteller

Monte Carlo Perturbation Calculations

- **MCNP & other Monte Carlo codes assume that the fission source distribution does not change even if a perturbation is introduced.**

- **That is, the fundamental eigenfunction is assumed constant, regardless of the perturbation.**

- **This approximation can lead to significant errors in perturbation theory estimates**

- **Accounting for source-shape changes in Monte Carlo perturbation theory can be an important effect**

- **Reported in**

  Y.Nagaya & T.Mori, "Evaluation of Perturbation Effect Due to Fission-Source Change in Eigenvalue Problems by Monte Carlo Methods," PHYSOR-2000 (2000).

  Y. Nagaya & F.B. Brown, "Estimation of Change in Keff due to Perturbed Fission Source Distribution in MCNP", M&C Topical, Gatlinburg (2003)

  Y. Nagaya & F.B. Brown, "Implementation of a Method to Estimate Change in Eigenvalue Due to Perturbed Fission Source Distribution into MCNP", LA-UR-03-1387 (2003).

- Central perturbation

Godiva Fission Distributions
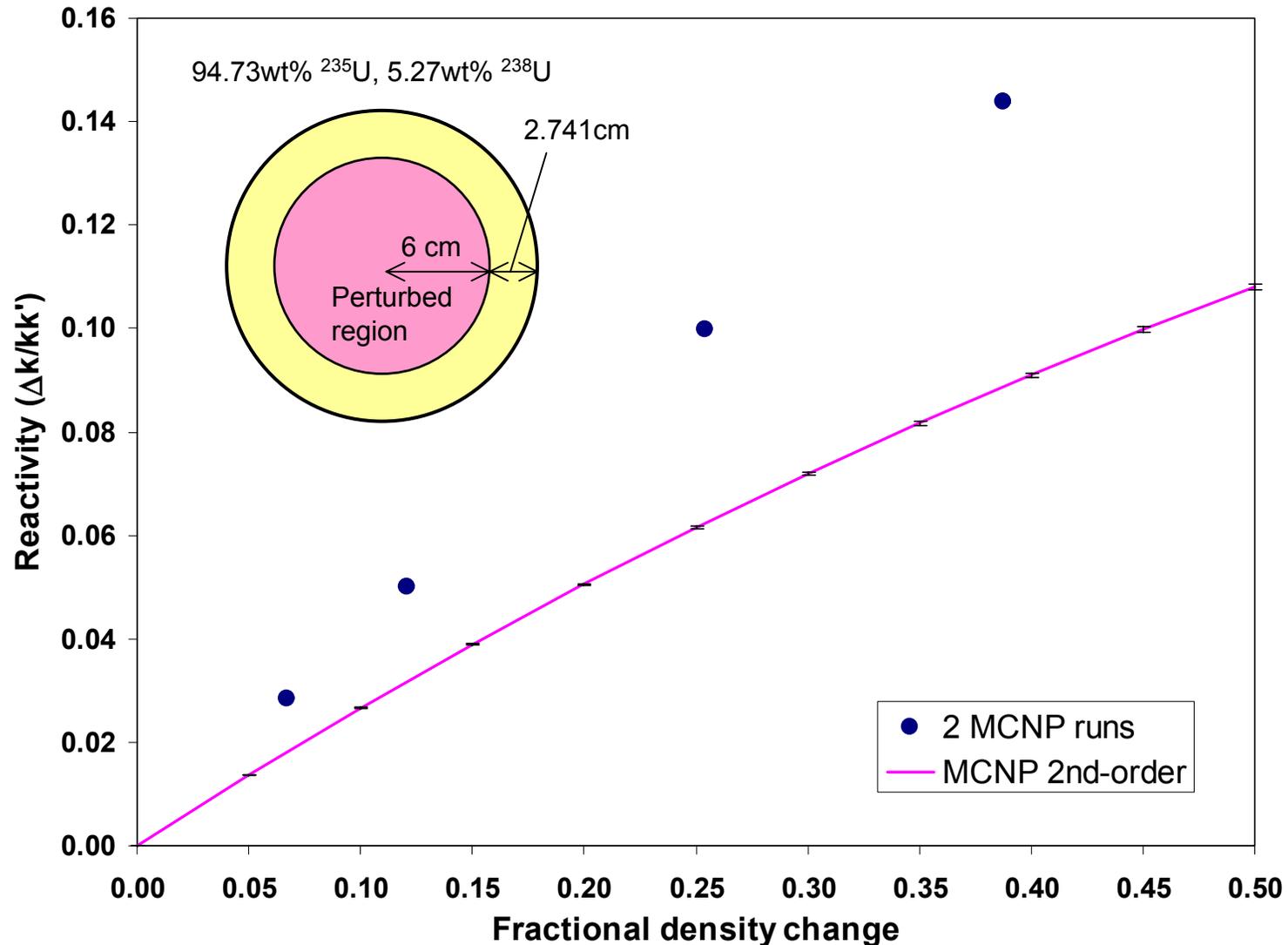
- Normalized fission source distributions - initial & perturbed

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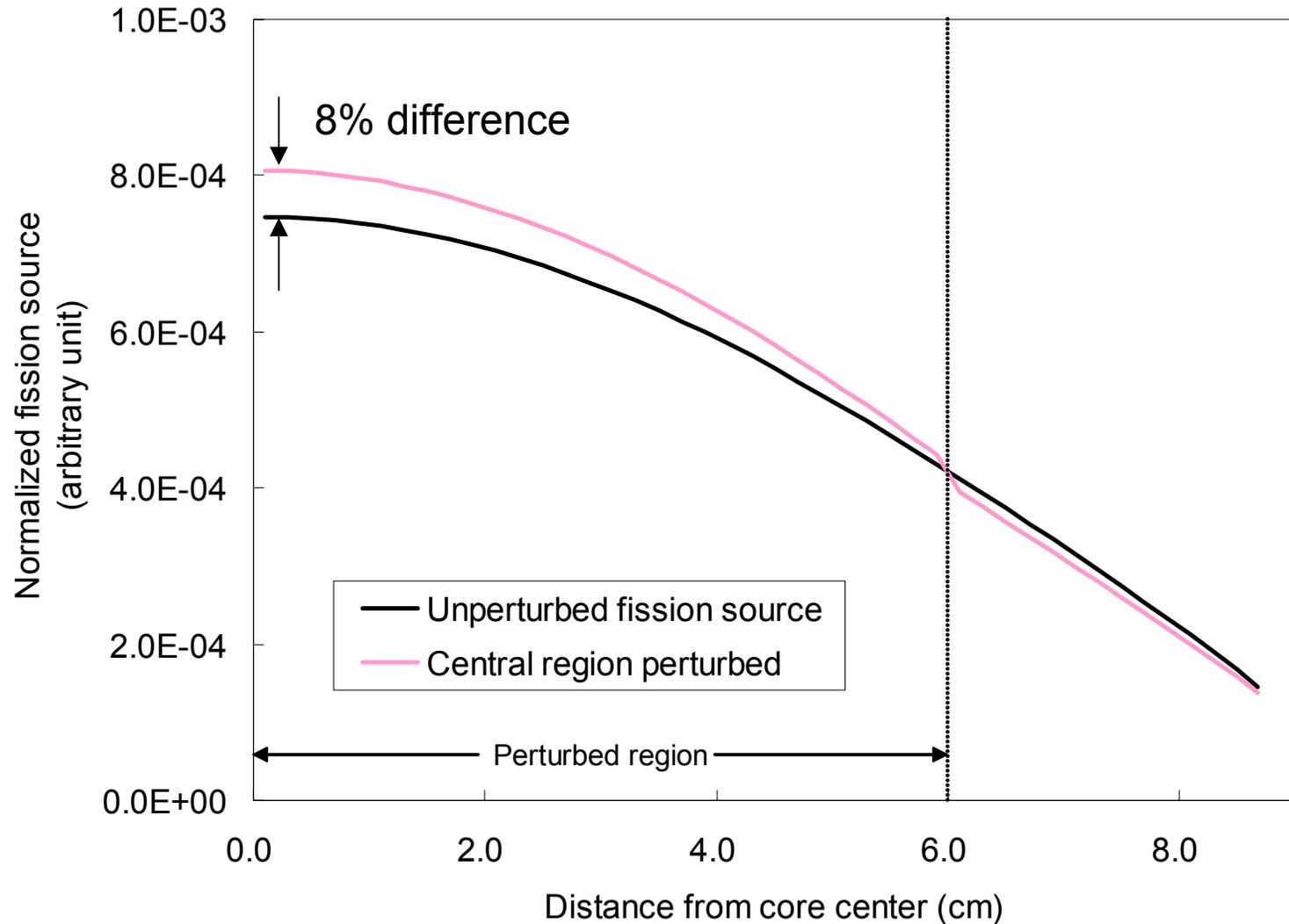
- Change in k can be expressed by the Taylor series expansion.

$$\Delta k = \frac{\partial k}{\partial a}\Delta a + \frac{1}{2}\frac{\partial^2 k}{\partial a^2}(\Delta a)^2 + \cdots + \frac{1}{n!}\frac{\partial^n k}{\partial a^n}(\Delta a)^n + \cdots$$

a : fractional change in a perturbation parameter

First-order
differential
coefficient

$$\frac{\partial k}{\partial a} = \frac{\int dP \int dP' \frac{\partial}{\partial a}\left[K_F(P;P')S_f(P')\right]}{\int dP' S_f(P')}$$

Second-order
differential
coefficient

$$\frac{\partial^2 k}{\partial a^2} = \frac{\int dP \int dP' \frac{\partial^2}{\partial a^2}\left[K_F(P;P')S_f(P')\right]}{\int dP' S_f(P')}$$

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$$\frac{\partial k_o}{\partial a} = \frac{1}{\iiint S_f dr_0 dE_1 d\Omega_1} \sum_{m=1}^{\infty} \int dP_m \cdots \int dP_1 \int dr_0 \left[\sum_{\ell=1}^{m} \left(\frac{1}{C_{f,\ell}} \frac{\partial C_{f,\ell}}{\partial a} + \frac{1}{T_\ell} \frac{\partial T_\ell}{\partial a} \right.\right.$$

$$\left.\left. + \frac{1}{C_{s,\ell-1}} \frac{\partial C_{s,\ell-1}}{\partial a} + \frac{1}{T_{\ell-1}} \frac{\partial T_{\ell-1}}{\partial a} + \cdots + \frac{1}{T_1} \frac{\partial T_1}{\partial a} \right) \frac{\nu \Sigma_f}{\Sigma_t} W \right]$$

$$\times \tilde{\alpha}_m \tilde{T}_m \tilde{C}_{s,m-1} \tilde{T}_m \cdots \tilde{C}_{s,1} \tilde{T}_1 \tilde{S}_f$$

$$\frac{\partial k_s}{\partial a} = \frac{1}{\iiint S_f dr_0 dE_1 d\Omega_1} \sum_{m=1}^{\infty} \int dP_m \cdots \int dP_1 \int dr_0 \left[\sum_{\ell=1}^{m} \left(\frac{1}{S_f} \frac{\partial S_f}{\partial a} \right) \frac{\nu \Sigma_f}{\Sigma_t} W \right]$$

$$\times \tilde{\alpha}_m \tilde{T}_m \tilde{C}_{s,m-1} \tilde{T}_m \cdots \tilde{C}_{s,1} \tilde{T}_1 \tilde{S}_f$$

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First order differential coefficient for k

Additional weight

Fission collision kernel

$$\frac{\partial k}{\partial a} = \frac{1}{\iiint S_f dr_0 dE_1 d\Omega_1} \sum_{m=1}^{\infty} \int dP_m \cdots \int dP_1 \int dr_0 \left[\sum_{\ell=1}^{m} \left(\frac{1}{C_{f,\ell}} \frac{\partial C_{f,\ell}}{\partial a} + \frac{1}{T_\ell} \frac{\partial T_\ell}{\partial a} \right. \right.$$

$$\left. \left. + \frac{1}{C_{s,\ell-1}} \frac{\partial C_{s,\ell-1}}{\partial a} + \frac{1}{T_{\ell-1}} \frac{\partial T_{\ell-1}}{\partial a} + \cdots + \frac{1}{T_1} \frac{\partial T_1}{\partial a} + \frac{1}{S_f} \frac{\partial S_f}{\partial a} \right) \frac{\nu \Sigma_f}{\Sigma_t} W \right]$$

$$\times \widetilde{\alpha}_m \widetilde{T}_m \widetilde{C}_{s,m-1} \widetilde{T}_m \cdots \widetilde{C}_{s,1} \widetilde{T}_1 \widetilde{S}_f$$

→ Fission source

→ Scattering collision kernel

→ Transport kernel

→ Absorption probability

Perturbed source effect

Collision estimate for k

Composition : 94.73wt% ^{235}U, 5.27wt% ^{238}U
Vacuum boundary condition

2.741cm

8.741cm

6 cm
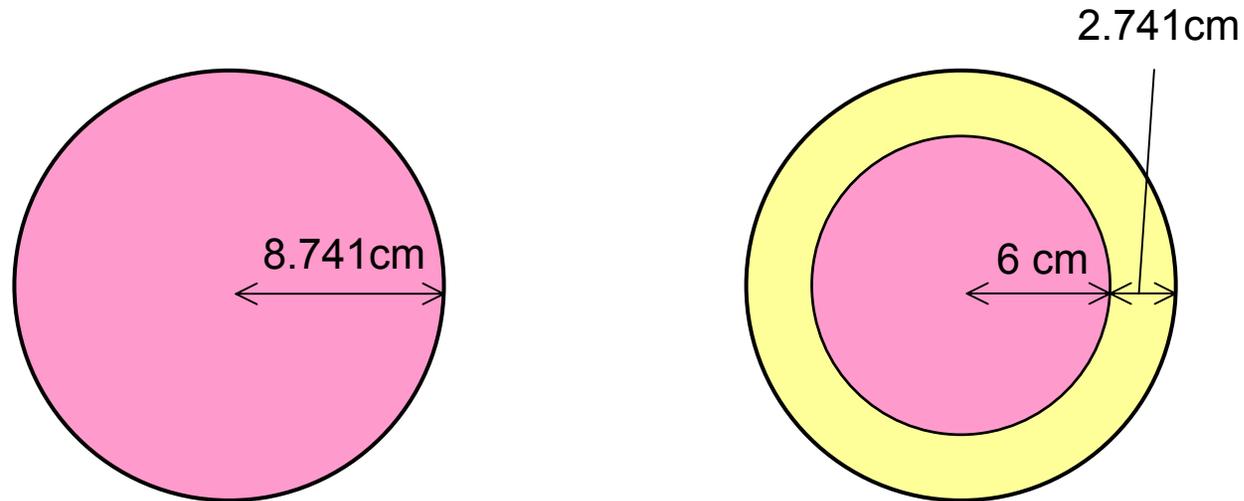
Perturbed Region (density change)

(a) Uniform perturbation   (b) Central perturbation

Uniform perturbation

Central perturbation

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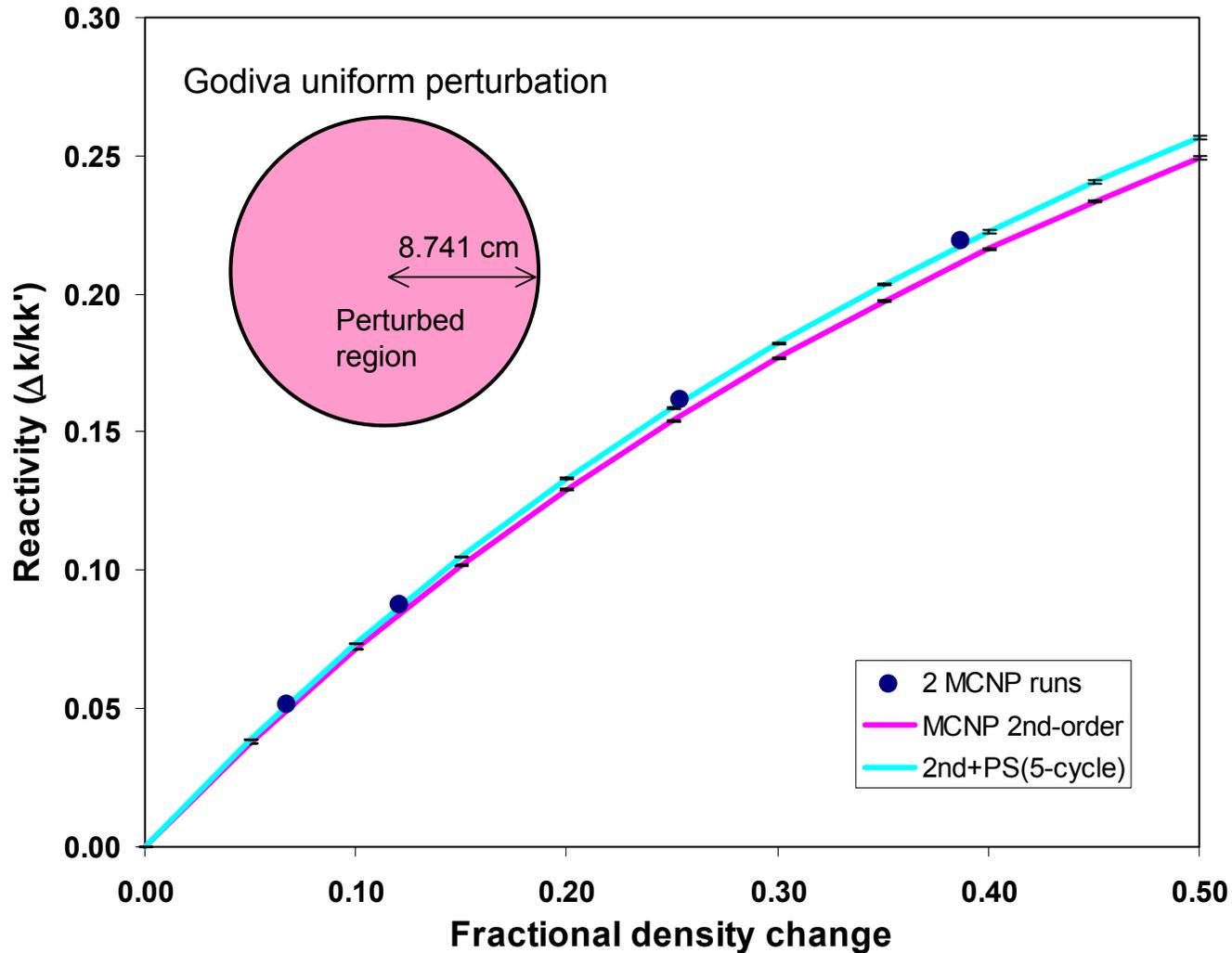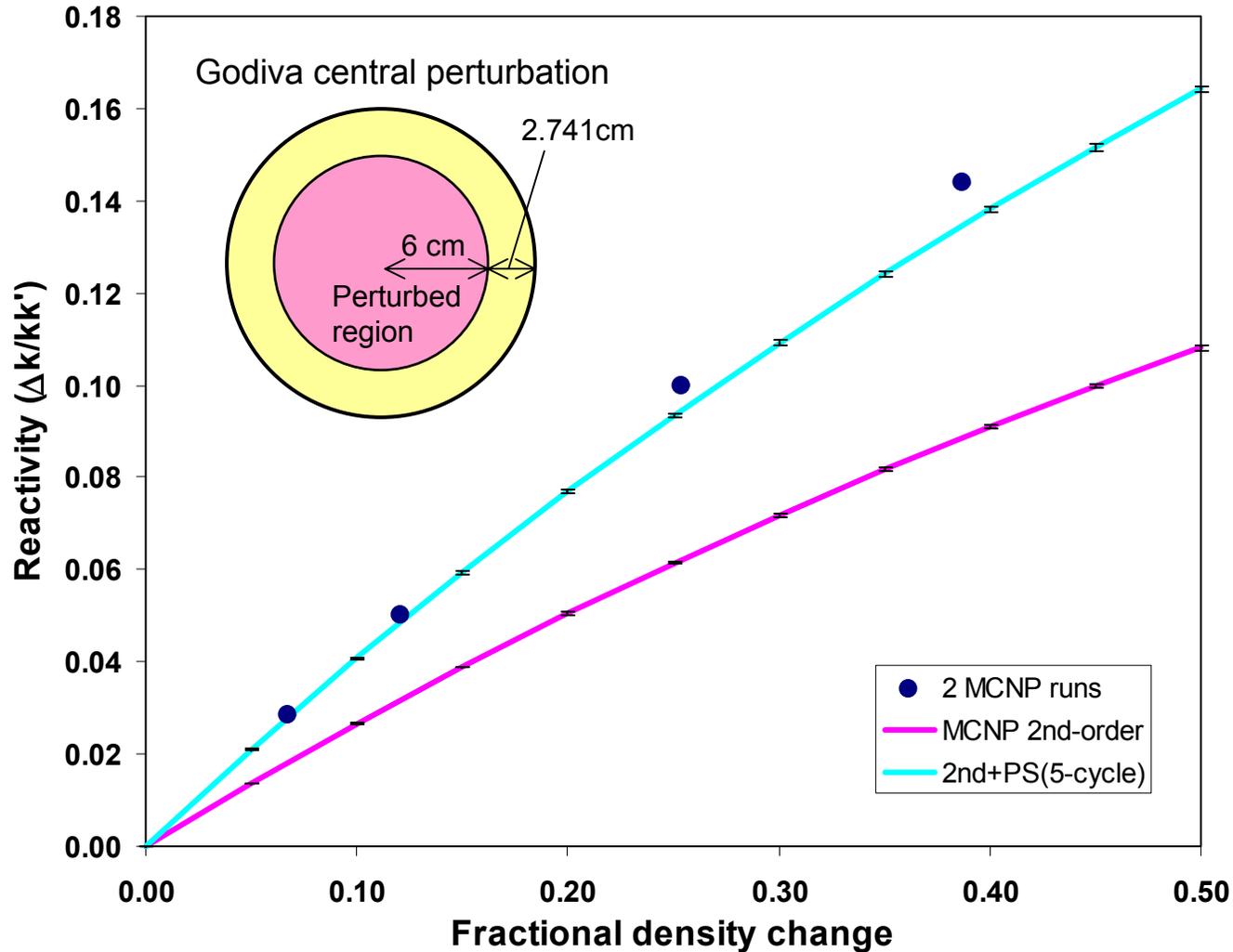
Automated Variance Reduction:

MCNP5
+
Deterministic Adjoint

Jeremy Sweezy, Tom Booth, Forrest Brown,

Joe Chiaramonte (Schlumberger)

- **Development of an Automated Variance Reduction Method for MCNP5 is underway**

- **MCNP combinatorial geometry is converted to PARTISN mesh geometry**
  - **PARTISN is LANL's 2D/3D discrete-ordinates code**
  - **Uses Weight-Window-Generator mesh**
  - **Not adaptive (for now)**

- **Adjoint fluxes from PARTISN used to generate weight windows**
  - **Option for angular weight windows (as in AVATAR)**
  - **Option for automatic source energy biasing**

- **Weight Window mesh plotting capability**

**MCNP5
combinatorial
geometry**
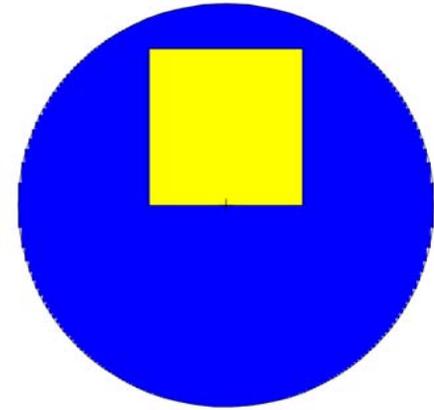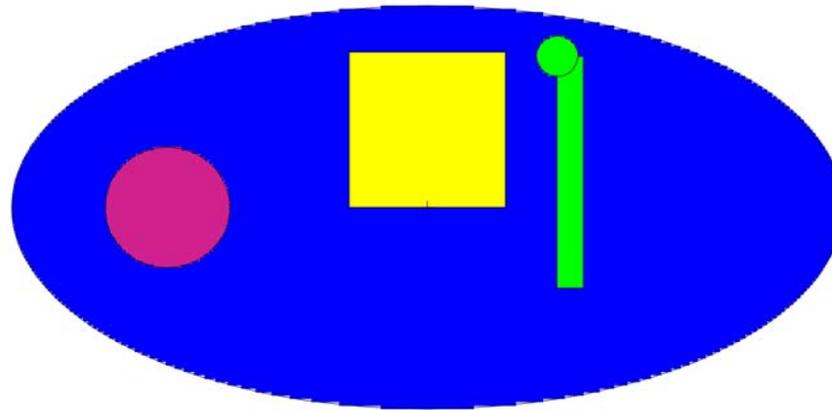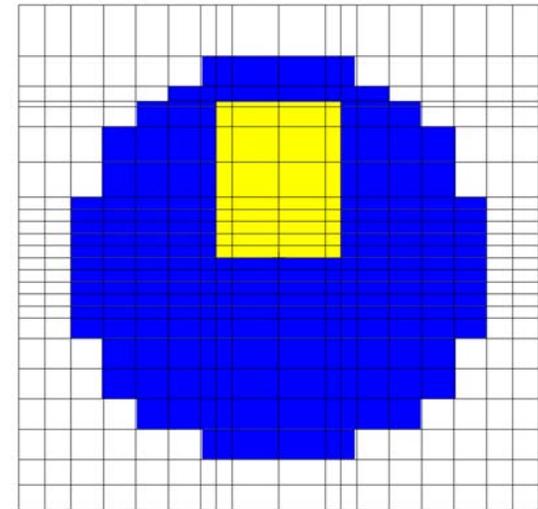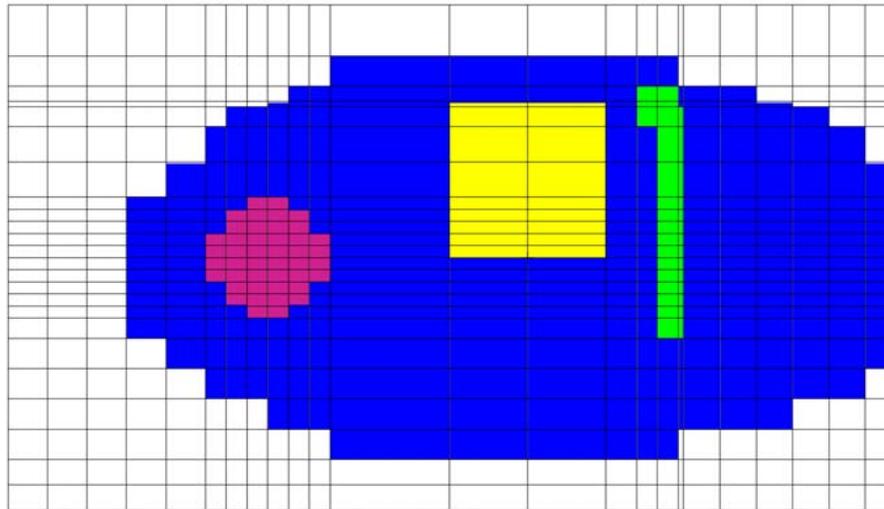
**PARTISN
mesh
geometry**

**MCNP5
combinatorial
geometry**

**PARTISN
mesh
geometry**

Standard MCNP WWG

Deterministic WWG
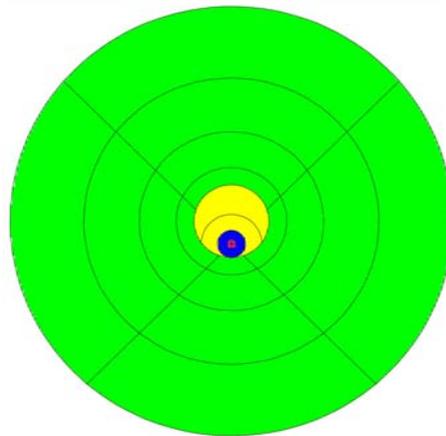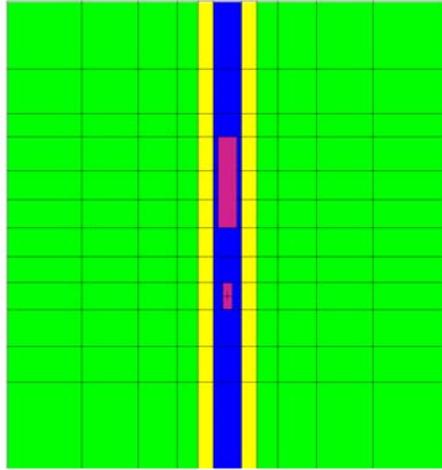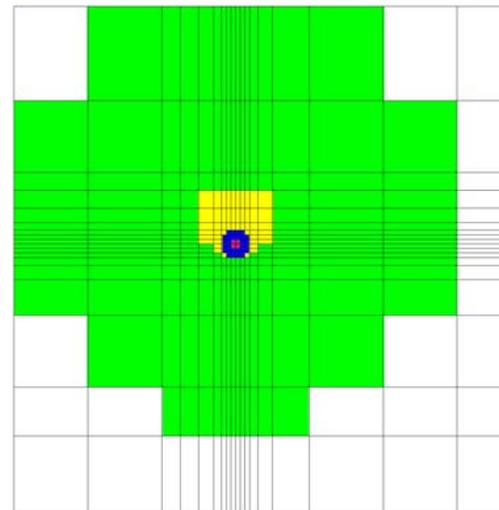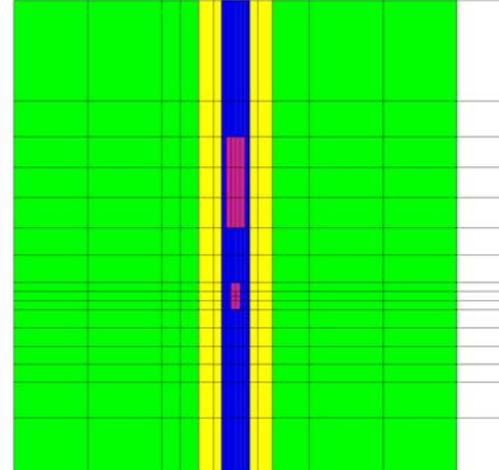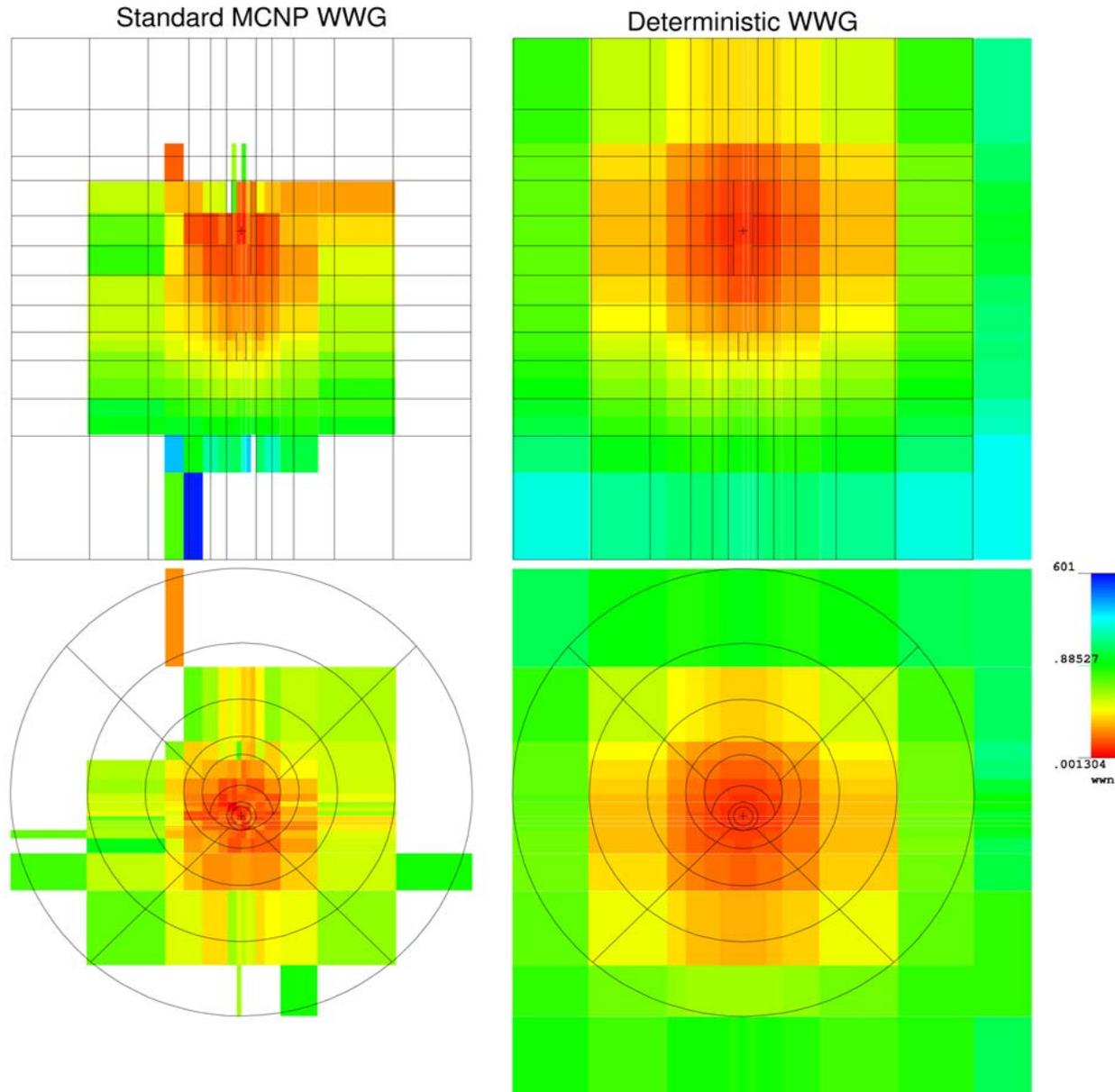
FOM vs. WWG time
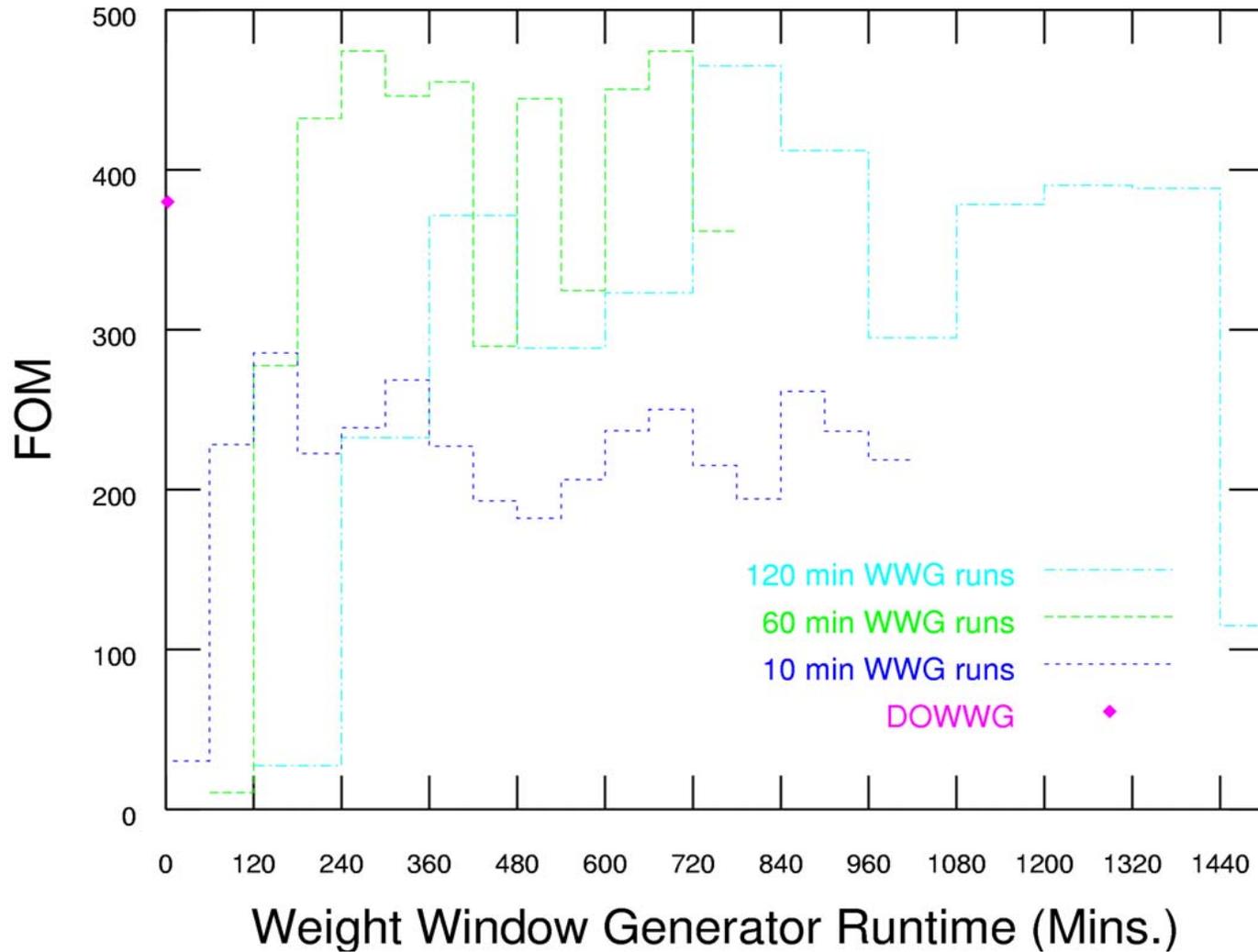
- Cf-252 Source

- 100-cm Polyethylene Shield

- Measuring Neutron Dose

- In 5-meter room with 61-cm thick concrete walls.
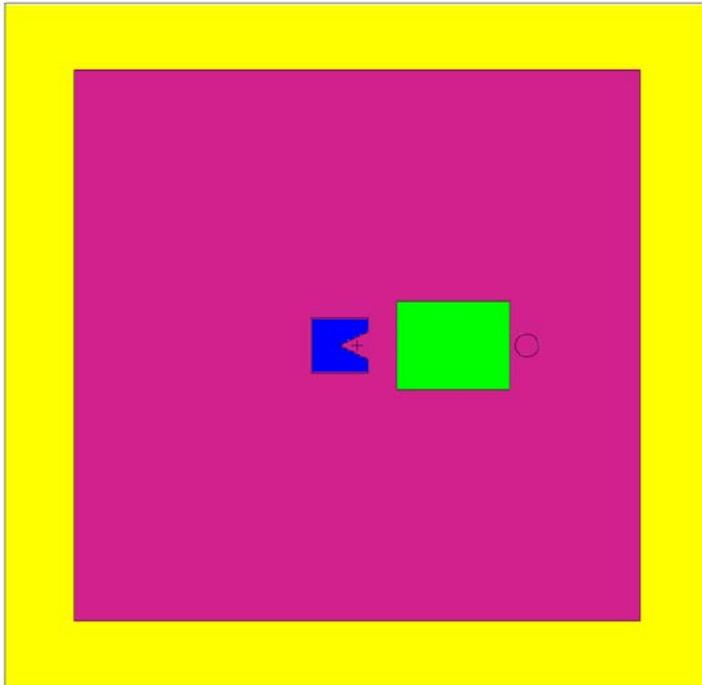
X-Y   X-Z
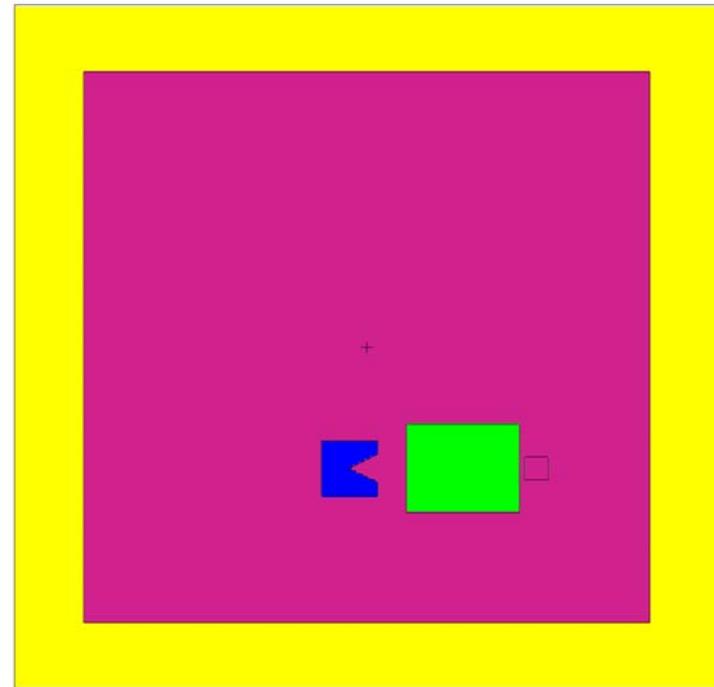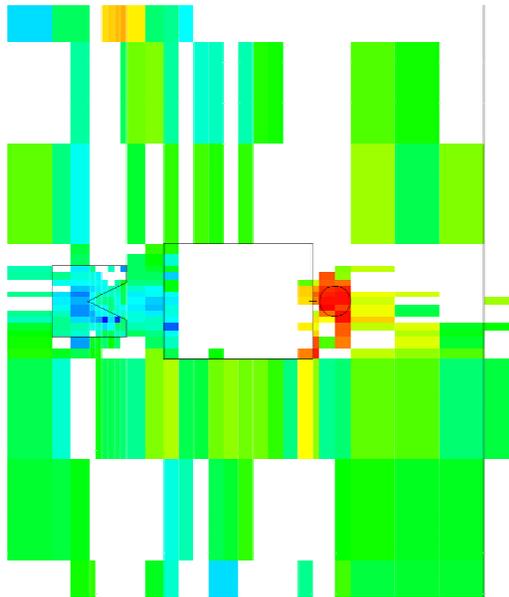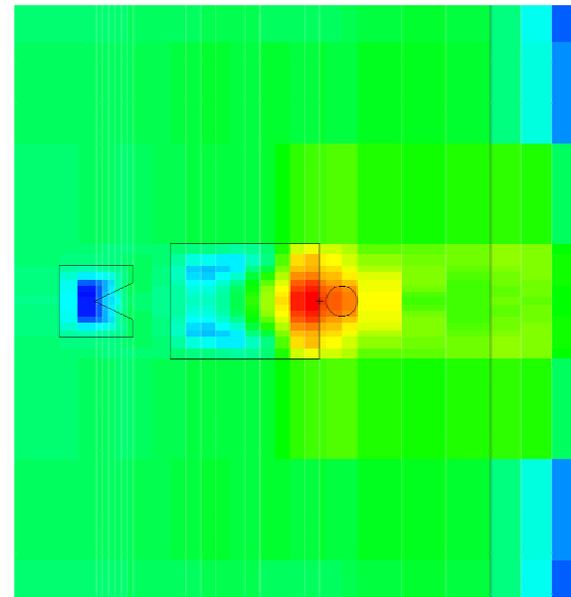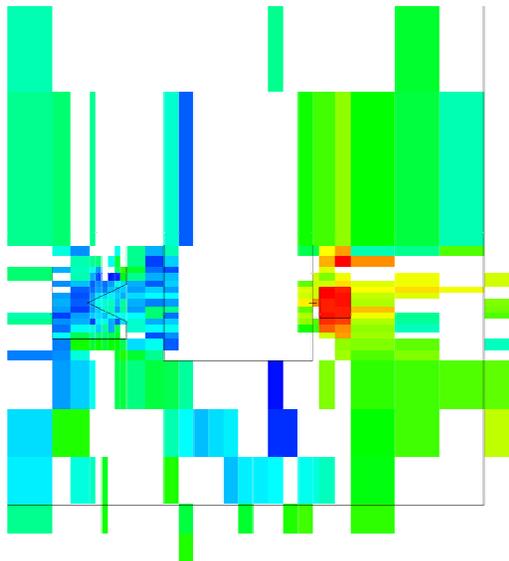
FOM vs. WWG time

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**Diagnostics
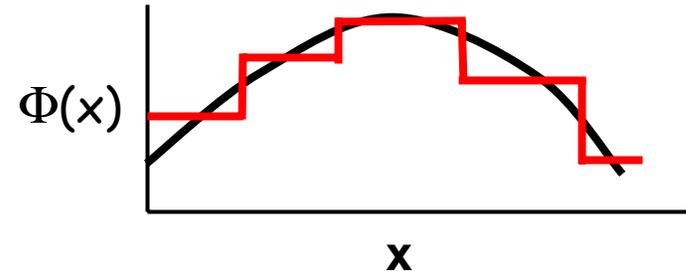Applications
Group (X-5)**

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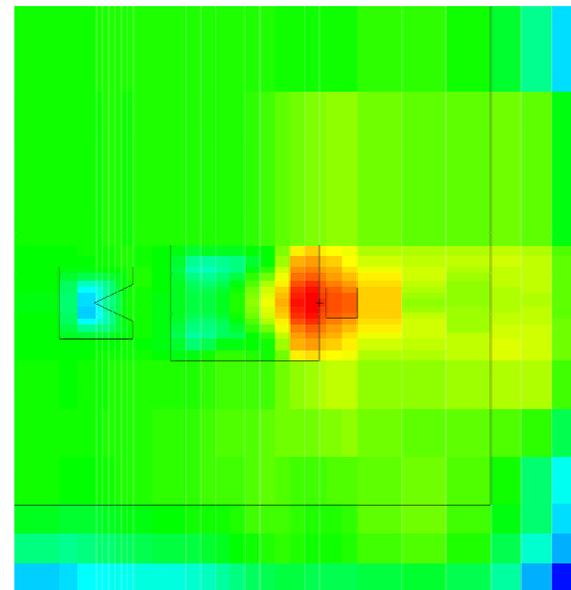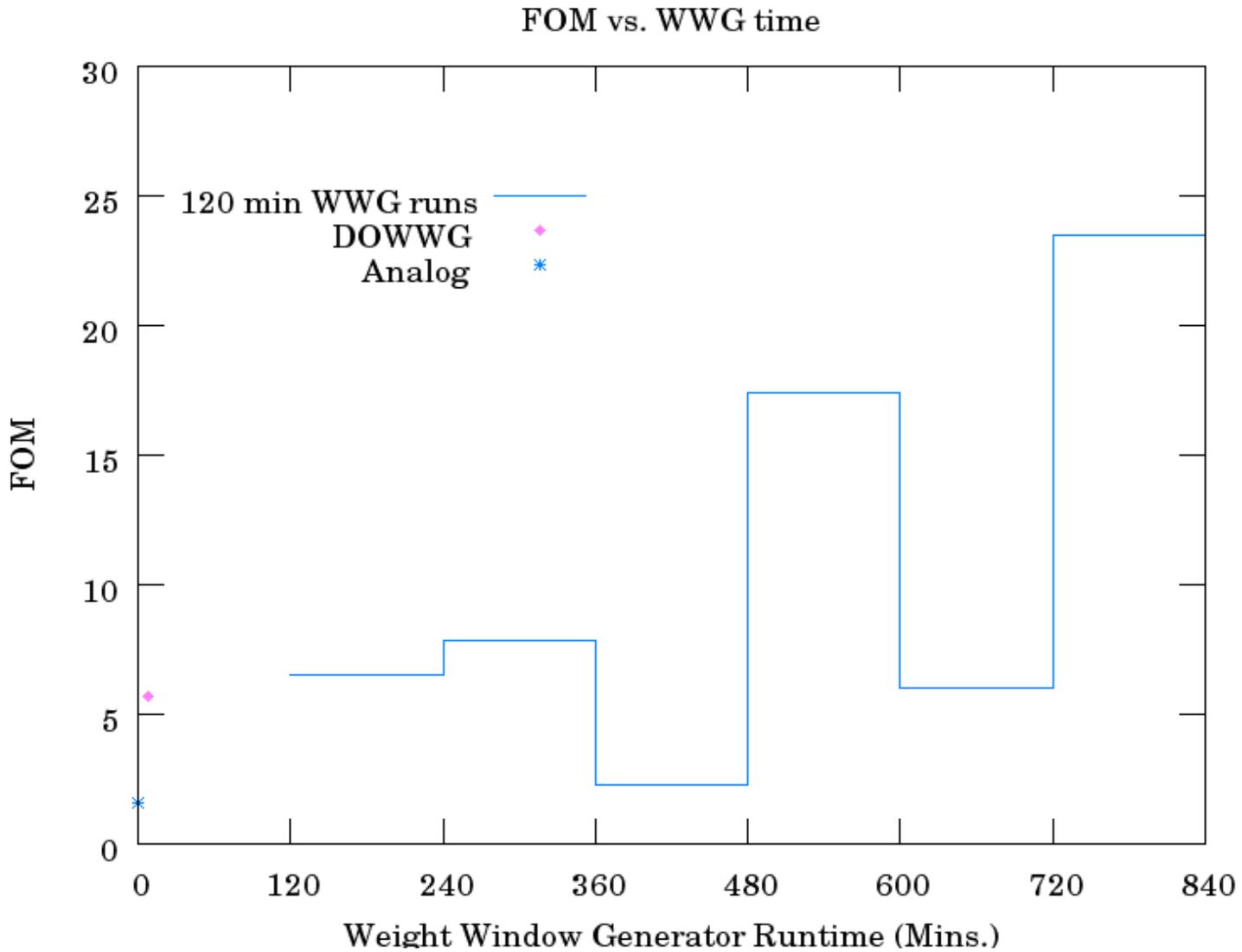
Continuously Varying Tallies

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[See papers for PHYSOR-2004]

Continuously Varying Tallies

- **Conventional Monte Carlo codes tally integral results**
  - **Tallies summed into bins**
  - **Zero-th order quantities**
  - **Stepwise approximation to results** $\Phi(x)$

x

- **Higher order tallies**
  - **Represent results by high-order, orthogonal polynomial expansion within each cell**
  - **Make tallies for expansion coefficients**
  - **Legendre polynomial representation for continuous tallies**

$$\Phi(x) = \sum_{n=0}^{N} \frac{2n+1}{2} \cdot b_n \cdot P_n \left[\frac{2}{\Delta x}(x - x_{\min}) - 1 \right]$$

$$b_n = \frac{2}{\Delta x} \int_{x_{\min}}^{x_{\max}} \Phi(x) P_n \left[\frac{2}{\Delta x}(x - x_{\min}) - 1 \right] dx$$

- **Make tallies for the Legendre coefficients at each collision or flight:**

$$b_n = \frac{2}{\Delta x} \int_{x_{\min}}^{x_{\max}} \Phi(x) P_n \left[\frac{2}{\Delta x} (x - x_{\min}) - 1 \right] dx$$
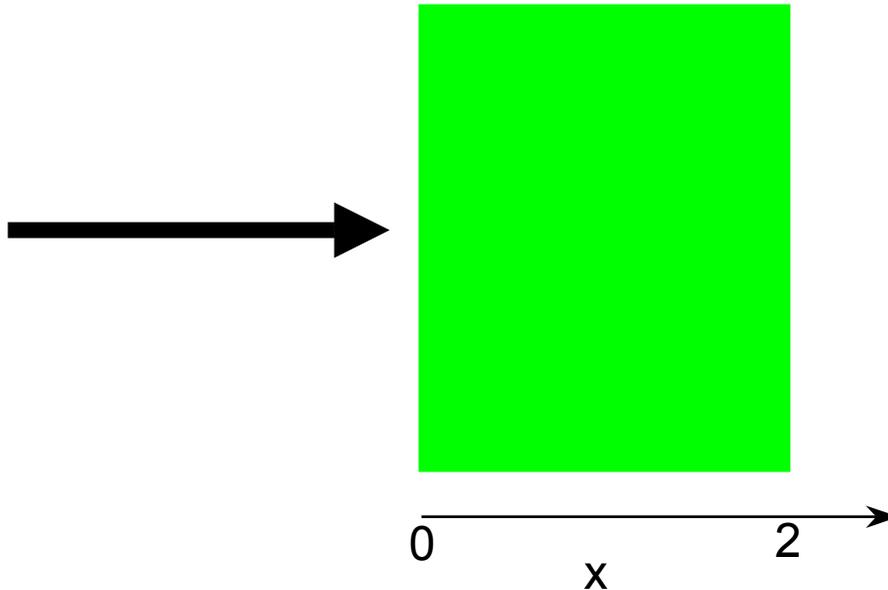
- **At collisions, tally** $\dfrac{wgt}{\Sigma_T} \cdot P_n \left[\dfrac{2}{\Delta x}(x - x_{\min}) - 1 \right]$ **for n=1..N**

- **At flights, tally** $wgt \cdot \dfrac{1}{\mu} \displaystyle\int_{x}^{x+s} P_n \left[\dfrac{2}{\Delta x}(x' - x_{\min}) - 1 \right] dx'$ **for n=1,N**

- **Reconstruct** $\Phi(x)$ **and** $\sigma_\Phi^2(x)$ **from tallied coefficients**

- **Beam source into slab**
  - Vacuum boundaries
  - Density in slab varies from 0 at edges to 10 at center
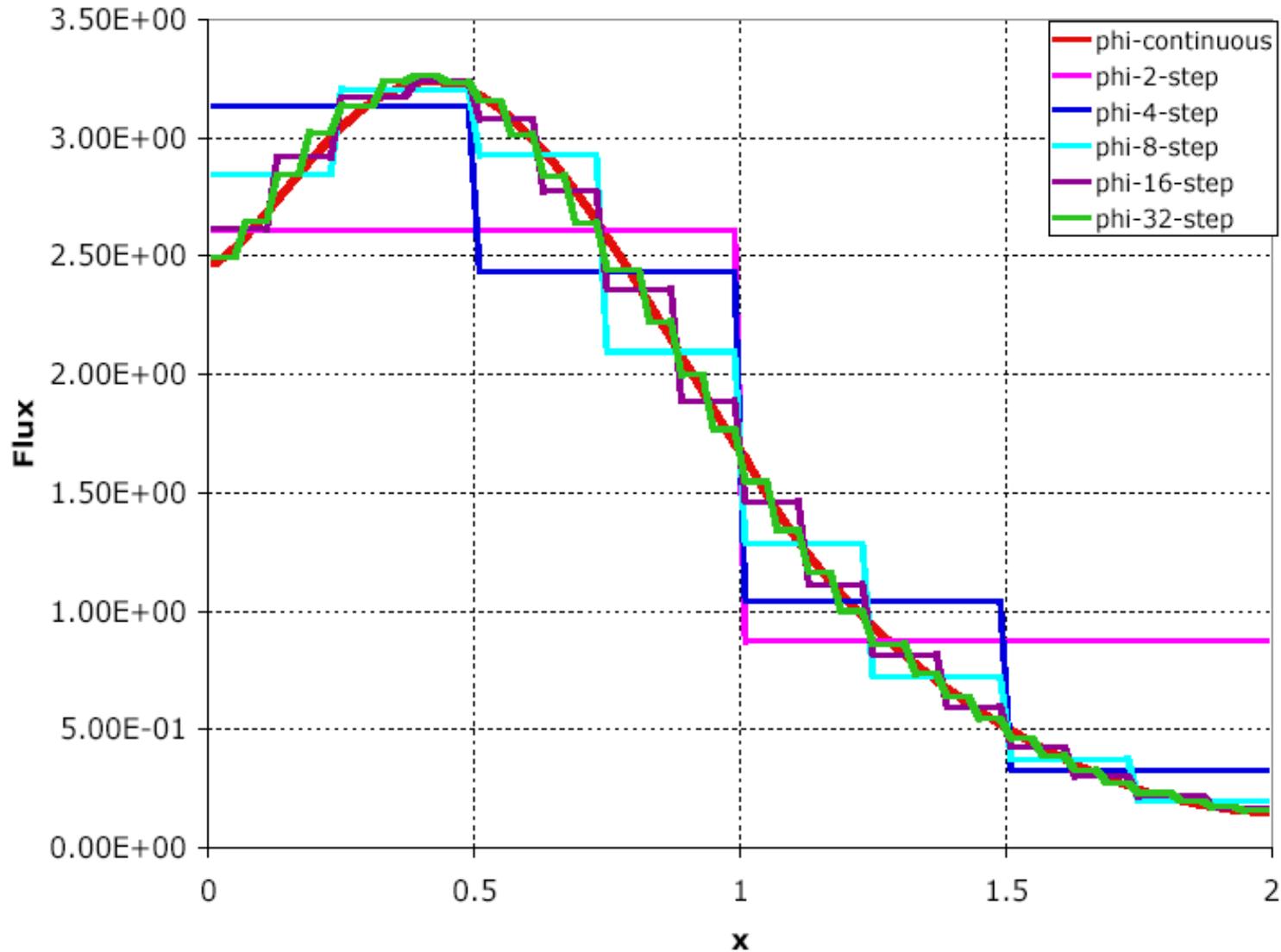 - $\Sigma_T = 1.00$, $\Sigma_s = 0.99$, $\Sigma_A = 0.01$

Figure 3. Flux results for Problem A: Beam into slab with linearly-varying density, continuous tally and various stepwise approximations

- **Eigenvalue calculation - depleted core with reflector**

  – Density varies quadratically in core: .25 at center, 2.25 at edges

  – Constant density in reflector, 1.0

  – Core: $\Sigma_T = 2.00$, $\Sigma_s = 0.125$, $\Sigma_A = 1.025$, $\Sigma_F = 0.85$, $\nu = 2.4$

  – Reflector: $\Sigma_T = 0.25$, $\Sigma_s = 0.24$, $\Sigma_A = 0.01$

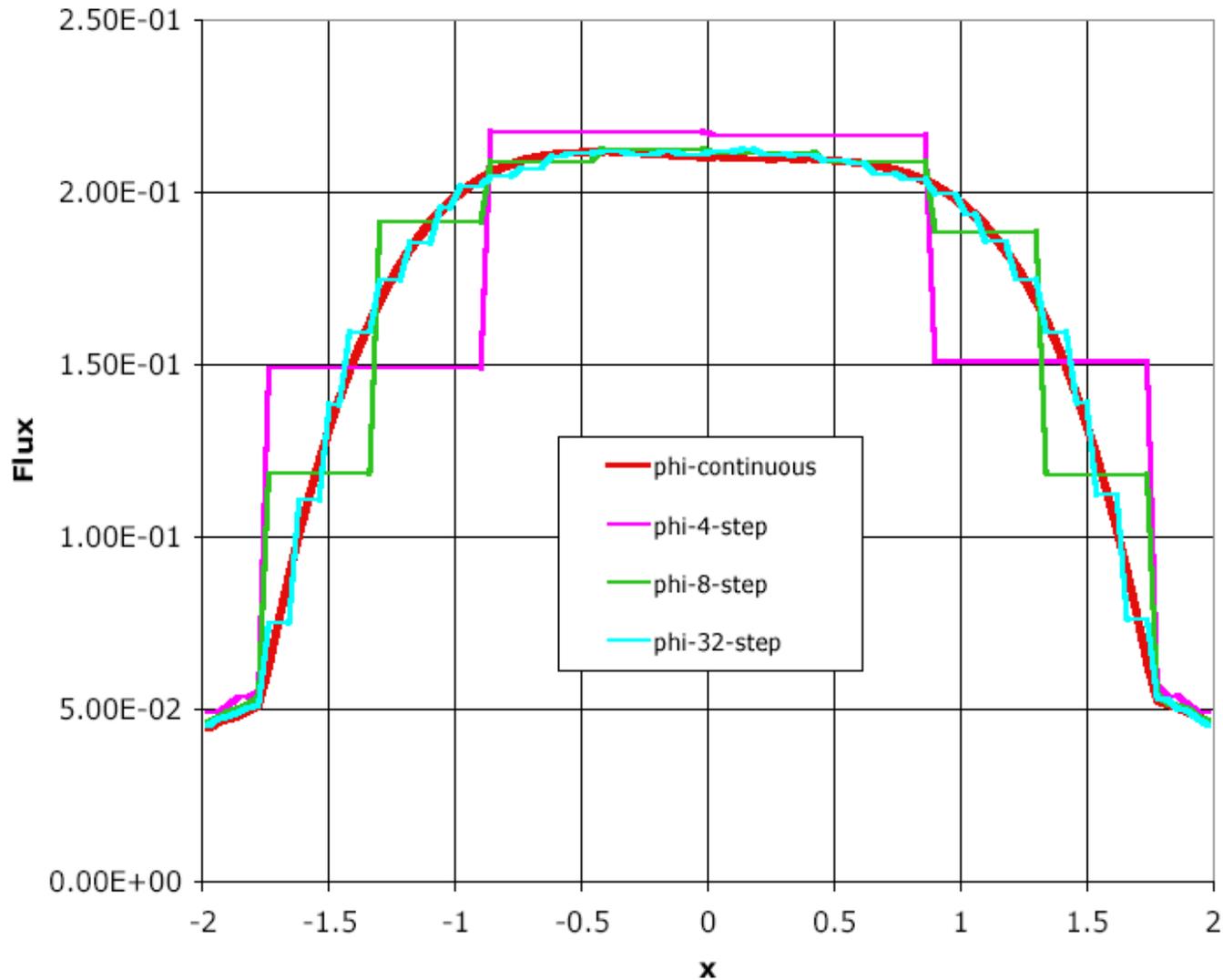-2 -1.75   1.75 2

X

Figure 4. Flux results for Problem B: Quadratic density variation, continuous tallies and various stepwise approximations
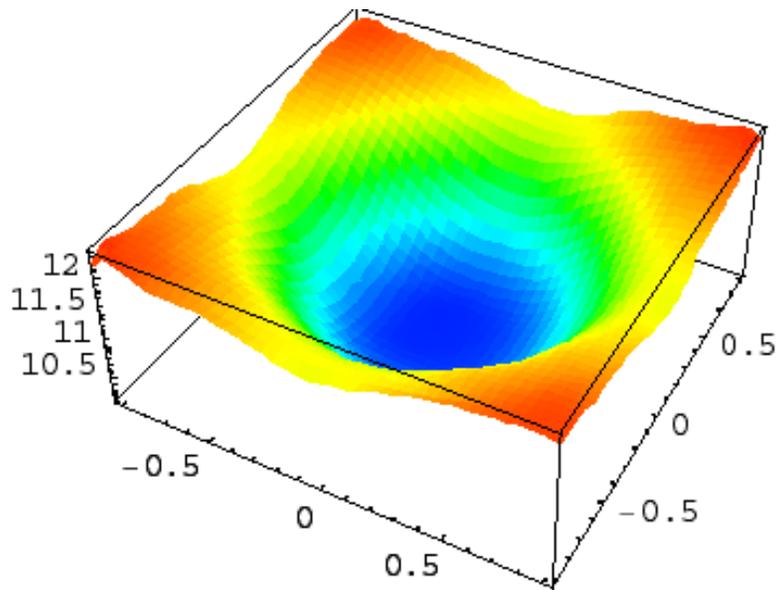
Figure 2a. 9x9 Legendre expansion tally for thermal neutron flux across the fuel pin obtained in a 2 million history simulation.
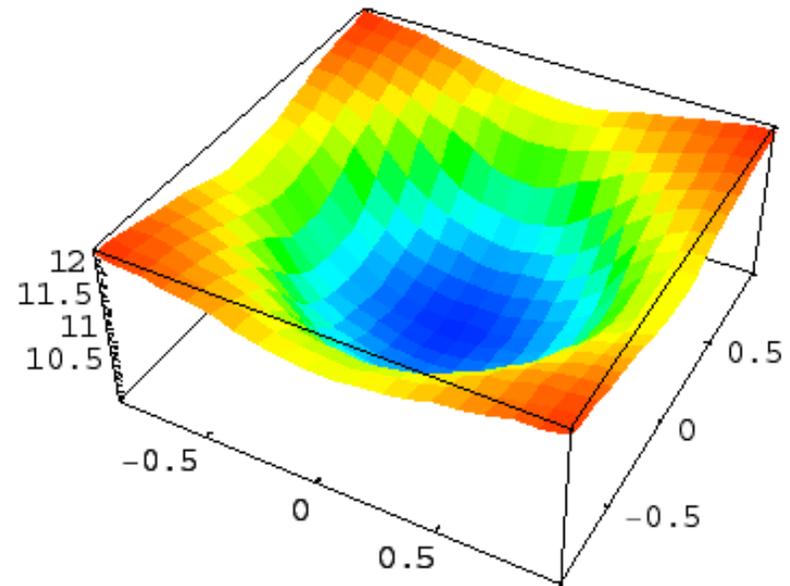
Figure 2b. MCNP5 20×20 mesh tally for thermal neutron flux across the fuel pin obtained in a 2 million history simulation.

- FB Brown, D Griesheimer, & WR Martin, "Continuously Varying Material Properties and Tallies for Monte Carlo Calculations", PHYSOR-2004, Chicago, IL (April, 2004)

- FB Brown & WR Martin, "Direct Sampling of Monte Carlo Flight Paths in Media with Continuously Varying Cross-sections", ANS Mathematics & Computation Topical Meeting, Gatlinburg, TN (April, 2003).

- DP Griesheimer & WR Martin, "Estimating the Global Scalar Flux Distribution with Orthogonal Basis Function Expansions", Trans. Am. Nucl. Soc. 89 (Nov, 2003)

- DP Griesheimer & WR Martin, "Two Dimensional Functional Expansion Tallies for Monte Carlo Simulations," PHYSOR-2004, Chicago, IL (April, 2004)

- ER Woodcock, T Murphy, PJ Hemmings, TC Longworth, "Techniques Used in the GEM Code for Monte Carlo Neutronics Calculations in Reactors and Other Systems of Complex Geometry," *Proc. Conf. Applications of Computing Methods to Reactor Problems*, ANL-7050, p. 557, Argonne National Laboratory (1965).

- LL Carter, ED Cashwell, & WM Taylor, "Monte Carlo Sampling with Continuously Varying Cross Sections Along Flight Paths", *Nucl. Sci. Eng.* **48**, 403-411 (1972).

- J. Spanier, "Monte Carlo Methods for Flux Expansion Solutions of Transport Problems," Nucl. Sci. Eng., **133**, 73 (1999).

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