Monte Carlo Methods Development and Related Research at the University of Michigan

Bill Martin

Nuclear Engineering and Radiological Sciences

University of Michigan

wrm@umich.edu

Outline of Talk

- Acknowledgements
- A Quick Look at NERS
- Monte Carlo methods development
  - Using the chord length distribution functions to compute Dancoff factorsCoupled deterministic/Monte Carlo methods for VHTR analysis
  - "On the fly" Doppler broadening
  - Application of the kernel density estimator to fission source convergence and Monte Carlo tallies
  - Acceleration of Monte Carlo source convergence
  - Functional Monte Carlo for interface effects
  - Time-dependent photon transport Monte Carlo

Acknowledgements

- University of Michigan PhD students
  - Wei Ji (now at RPI)
  - Gokhan Yesilyurt
  - Kaushik Banerjee
  - Bryan Toth
  - Emily Wolters
  - Jesse Cheatham
- Colleagues
  - John Lee
  - James Holloway
  - Forrest Brown (Los Alamos)
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  - NE/HP Fellowship
  - Naval Reactor Rickover Fellowship

Cooley Building

- 20 teaching faculty (2 F, 1 URM)
- 6 research faculty
- 116 undergraduates (25 F, 3 URM)
- 103 grad students (17 F, 5 URM)
- ~ $ 7M research/year
- #1 in 2008 USN&WR rankings for graduate programs in Nuclear Engineering

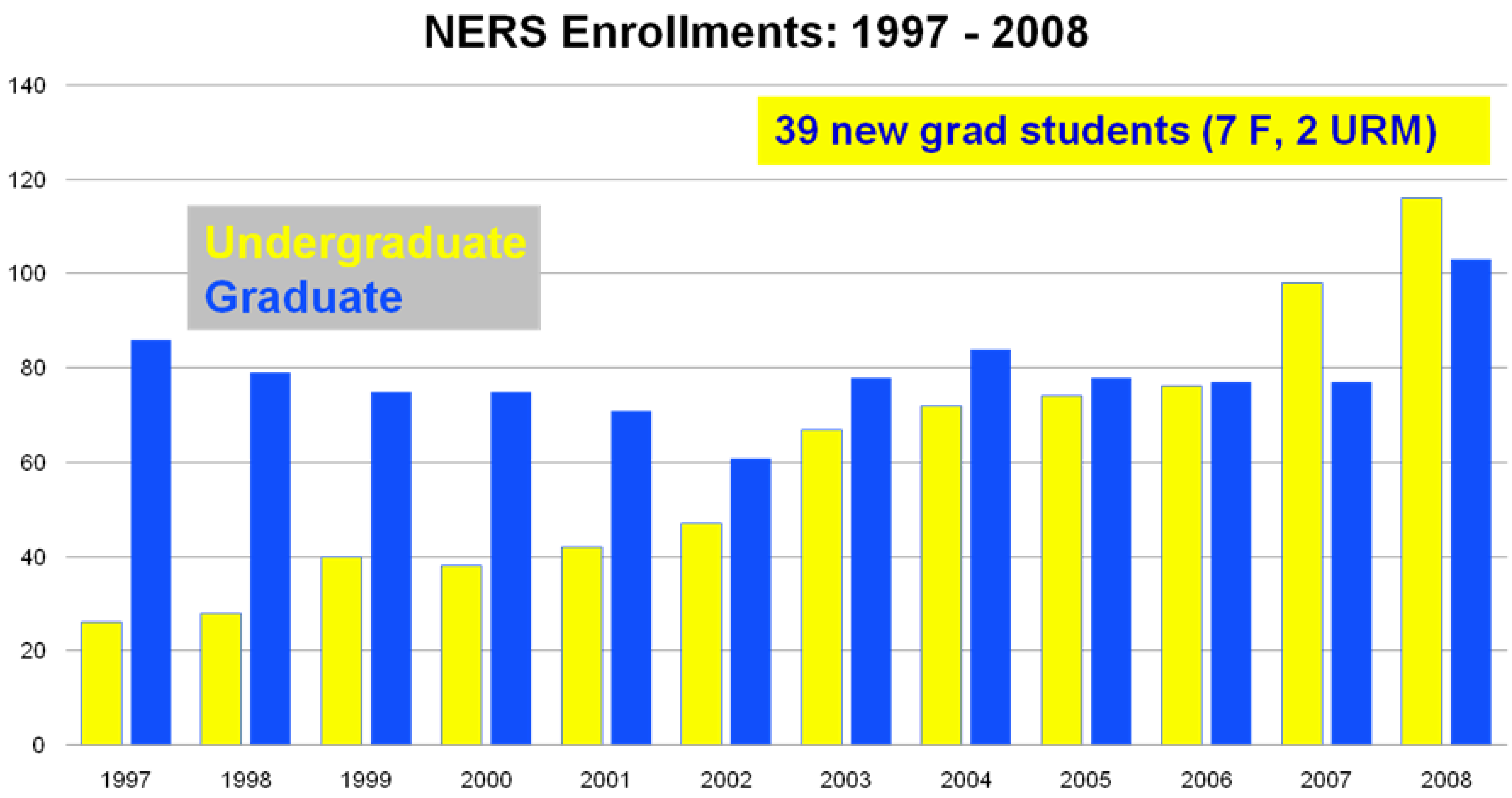
Snapshot of NERS: September 2008

History of NERS

- 1947: First UM course in nuclear energy applications offered.
- 1952: UM established first graduate program in Nuclear Engineering in the U.S.
- 1957: Ford Nuclear Reactor reached criticality. The FNR was the third university reactor and it operated successfully for 46 years before being shutdown in 2003.
- 1958: Department of Nuclear Engineering created as a graduate program. 50 years old last fall!
- 1965: Undergraduate program in Nuclear Engineering established.
- 1995: Department name changed to Nuclear Engineering and Radiological Sciences (NERS)

Vital Statistics

Enrollments



Degrees Awarded

- **Cumulative degrees awarded 1958-2008**
  - 708 BSE NERS
  - 205 BS Eng Phy
  - 1036 MS/MSE
  - 487 PhD
  - 9 Nuclear Engineer Professional Degrees

- **AY 2007-08 Degrees**
  - 30 BSE NERS
  - 8 BS Eng Phy
  - 14 MS/MSE
  - 9 PhD

- **Current enrollments**
  - NERS Undergraduate: 116
  - EP Undergraduate: 23
  - Graduate: 103

Quality Indicators

- **Undergraduate students**
- **Graduate students**
- **Faculty awards**
- **Department rankings**

Undergraduate Scholarships

- **11 National scholarships: $23k for AY07-08**
- **NERS funds 5 undergraduate scholarships**
  - **~ $30k/year**
  - **Endowments**

Graduate Fellowships

- **NERS graduate students have been awarded 31 national fellowships ~ $ 1 M/year**
  - ANS, DOE (including 2 Computational Science Fellows and 2 Rickover Fellows), NANT, NASA, HPS, DHS, NSF(2 NSF Fellowships)
- **Essentially all NERS graduate students are funded**
  - ~ 5 first-year students are self-funded or supported by their home countries (3 from Brazil Navy this year)
- **NRC Graduate Fellowships started in Fall 2008 ~ $100K/year**

Faculty Awards and Distinctions

National Academy of Engineering Member (2)

National Medal of Technology (1): Presidential Medal

***Fellows* of professional societies**

ANS (10), APS (7), IEEE (2), AIAA (1), AIMBE (1), AAAS (1), ASM (1), GSA (1), MSA (1), NACE (1), IOP (1)

NSF Presidential Young Investigator Awards (4)

E. O. Lawrence Award (2): U. S. Department of Energy

Arthur Holly Compton Award (5): American Nuclear Society

Glenn E. Murphy Award (3): American Society for Engineering Education

Tetalman Memorial Award: Society of Nuclear Medicine

Third Millennium Medal: 2000 IEEE members

Guggenheim Fellowship

Hawley Medal: Mineral Society of Canada

Reputation of the Department

National rankings: *U.S. News & World Report*

- Graduate: **#1** (2008) – back to #1!
- Undergraduate: **no ranking.** Nuclear Engineering is no longer ranked by *USN&WR* in the undergrad category

Students

- ***Mark Mills Award***: given annually by the American Nuclear Society to recognize the best technical paper based on a doctoral dissertation in nuclear engineering. **12** of the **45** annual awards have been awarded to UM doctoral graduates.

Faculty and Research

20 regular faculty, 5 research faculty, and 5 emeritus faculty have research interests in the following areas:

- **Fission systems and radiation transport**
- **Plasma physics and fusion**
- **Materials**
- **Radiation measurements and imaging**
- **Medical and health physics**

Fission Systems and Radiation Transport (6)

John Lee, Professor
- Reactor physics
- Space-time kinetics
-Fuel cycle analysis

Ed Larsen, Professor
- Computational particle transport
- Asymptotic methods
- Radiative transfer

James Holloway, Professor
- Computational physics
- Monte Carlo methods

Bill Martin, Professor
- Chair
- Computational particle transport
- Monte Carlo methods

Tom Downar, Professor
-Computational reactor physics
- Reactor safety

Alex Bielajew, Professor
Monte Carlo electron/photon transport

Plasma Physics and Fusion (5)

Ron Gilgenbach, Professor, EXPERIMENTS: e-beams, z-pinch, wave-generation, plasma propulsion, biological applications of intense radiation

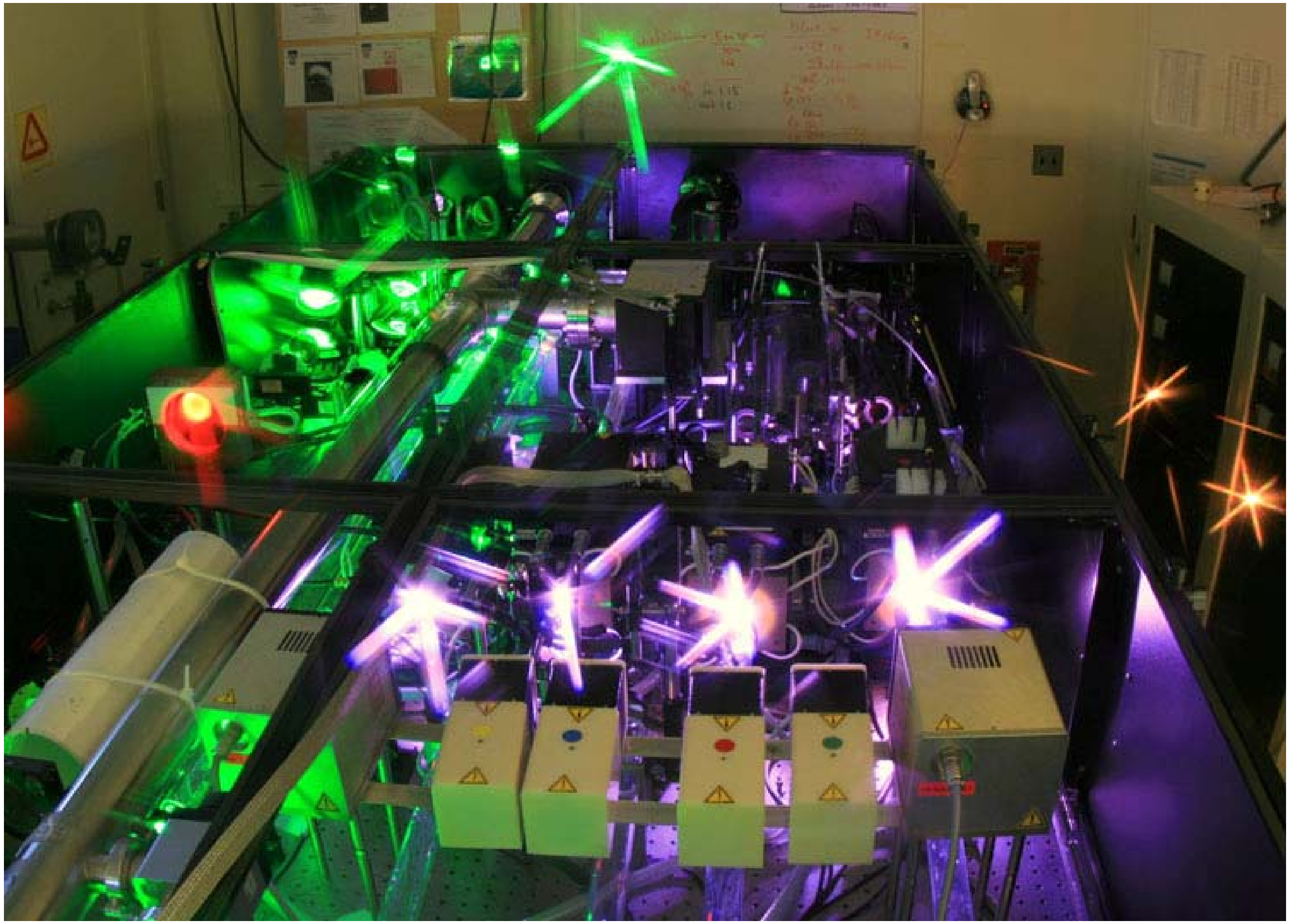
Y.Y. Lau, Professor, THEORY: e-beams, z-pinch, discharge, HPM sources, cathodes, nano-diodes, bio-theory

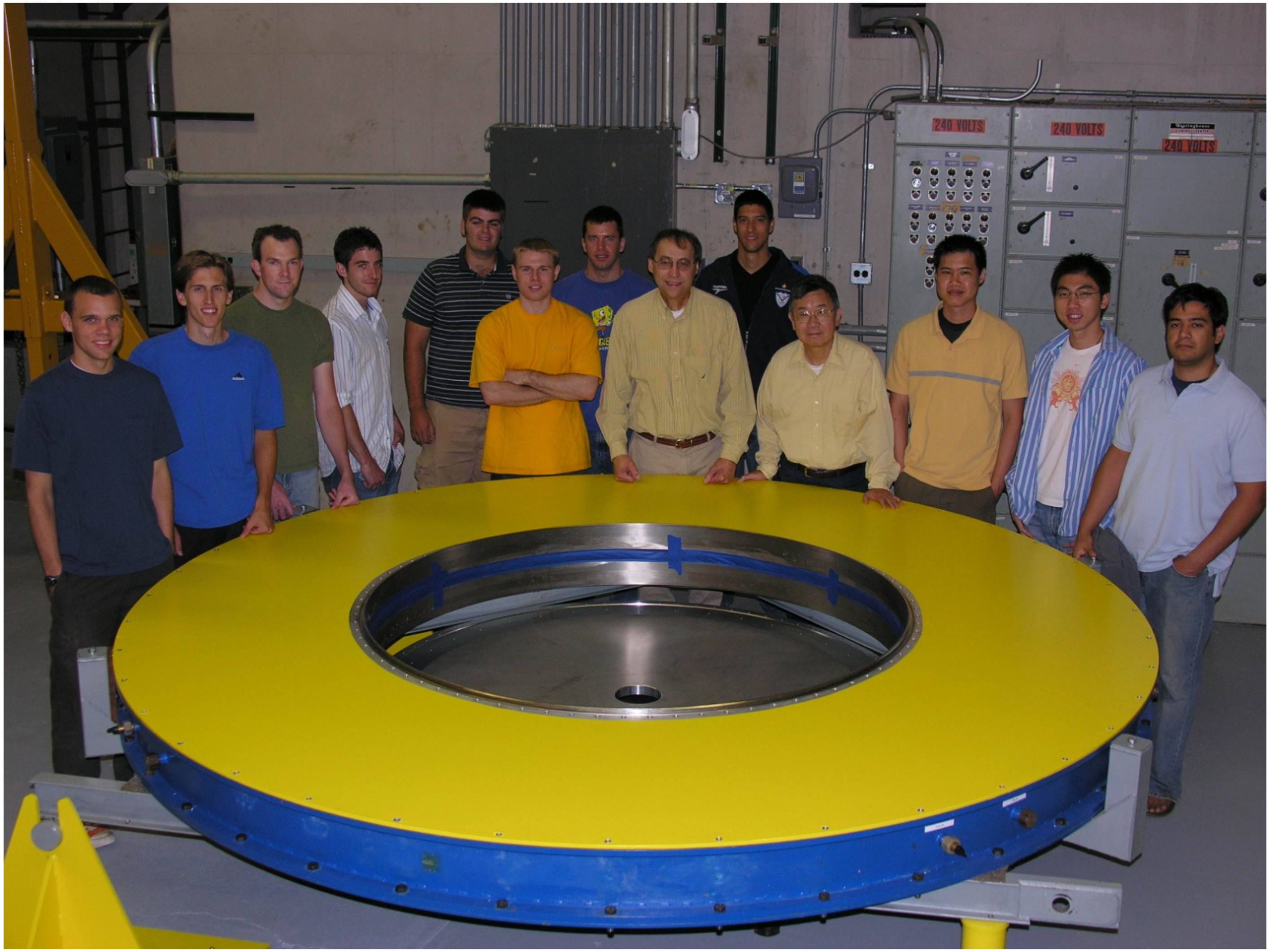
Karl Krushelnick, Professor, EXPERIMENTS: plasma physics, ultra-high intensity lasers, inertial confinement fusion, tabletop particle accelerators

John Foster, Associate Professor EXPERIMENTS: Space propulsion plasmas Materials processing plasmas Plasma-based approaches for environmental hazard mitigation

Alec Thomas, Assistant Professor, EXPERIMENTS: Fundamental high-field and plasma physics, laser-based fusion schemes, compact particle accelerators using lasers

Hercules laser in the Center for Ultrafast Optical Science (Karl Krushelnick)





Ron Gilgenbach and students with the 1-MA LTD machine, MAIZE, upon its arrival at the UM in 2008

UM Students and Faculty in Plasmas, Z-Pinches, Plasma Theory, Bioelectromagnetism & LTD Technology

Materials (4)

Gary Was, Professor

- Atomistic processes in materials
- Phase transformations in binary alloys during ion beam mixing
- Irradiation assisted stress corrosion cracking in stainless steels using high energy protons

Lumin Wang, Professor

- Transmission electron microscopy (TEM) study of microstructure evolution of solids during irradiation
- particle beam modification of materials

Michael Hartman, Assistant Professor

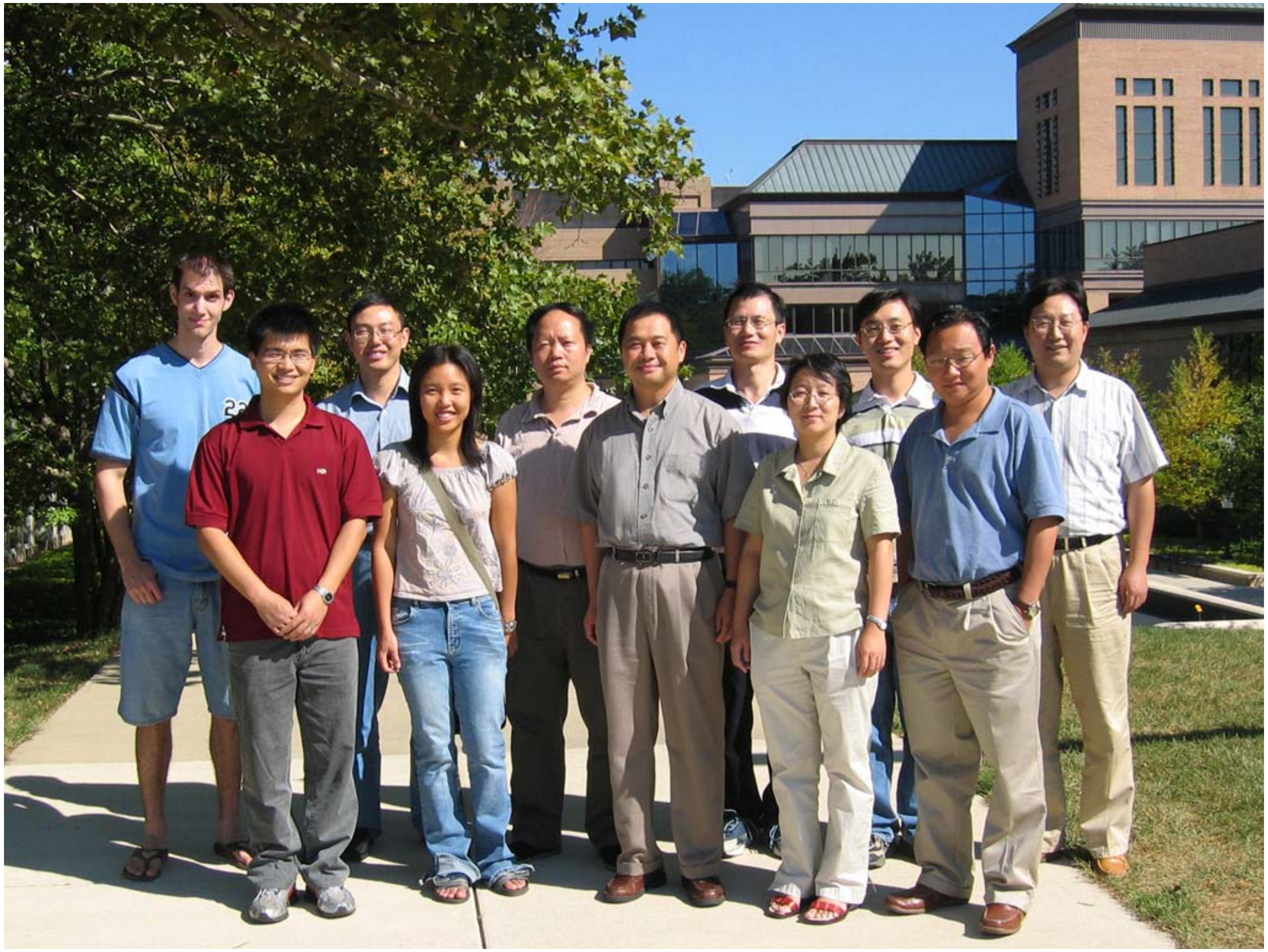
- Hydrogen storage for fuel cell applications
- Large scale hydrogen production systems

Michael Atzmon, Professor

-Nonequilibrium processes in materials
- Effect of radiation damage on structure of stainless steel
- Analysis and simulation

14 MeV D-T Neutron Generator in the Neutron Science Laboratory (Mike Hartman)

Lumin Wang's Research Group in NERS and MSE



Sponsored research:

- DOE BES: Self-organized 3-D array of nanostructures under irradiation
- DOE BES (with Ewing): Radiation effects in complex ceramic materials
- NSF NIRT (with Becker and Ewing): Nanoparticles in the environment
- Qynergy Corp (USAF): Evaluation of radiation effects in materials proposed for nuclear battery applications

Research areas: A. Radiation effects in nuclear engineering materials
B. Nanostructure processing with energetic particle beams

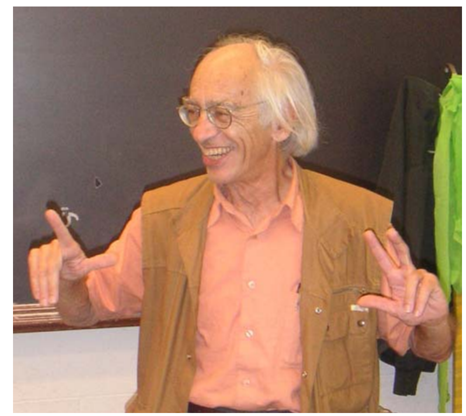
Radiation Measurements and Imaging (5)

David Wehe, Professor
- Radiation imaging
- Autonomous mobile robots

Kimberlee Kearfott, Professor
-Medical applications
- Personnel dosimetry

Zhong He, Professor
- Gamma-ray spectroscopy and imaging devices
-Room-temperature semiconductor gamma-ray spectrometers and imagers.

Sara Pozzi, Associate Professor
- Nuclear detection for non-proliferation



Ron Fleming, Professor
Spectroscopy/spectrometry of photons, neutrons, and charged particles

Detection for Nuclear Nonproliferation Group

Newly established group at the University of Michigan

Group Leader: Sara Pozzi

Group Members

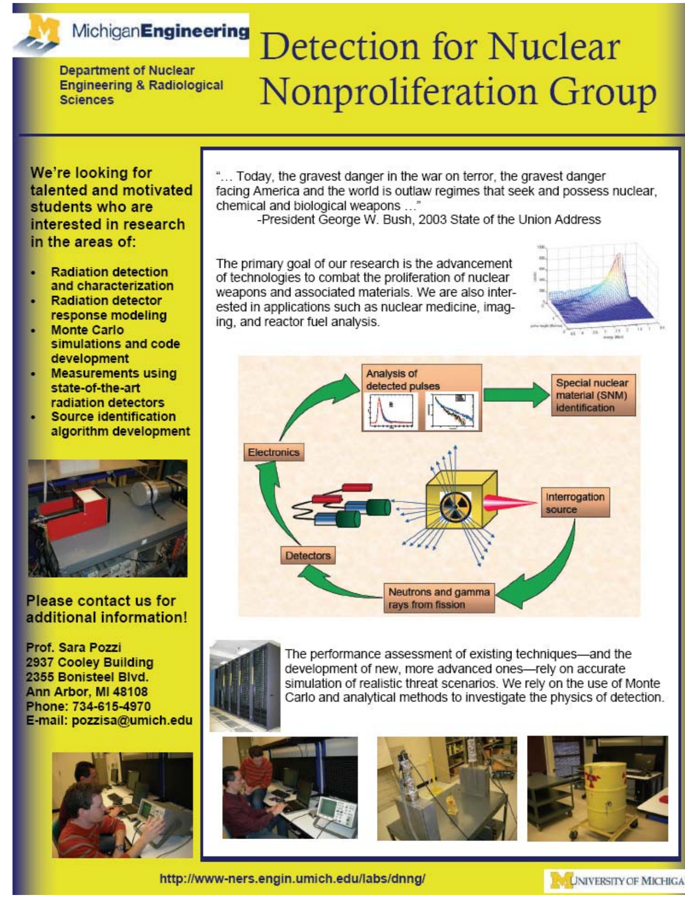
- Marek Flaska, Assistant research scientist
- Shaun Clarke, Postdoctoral researcher
- Eric Miller, Graduate student
- Jennifer Dolan, Graduate student
- Ben Maestas, Graduate student
- Mark Bourne, Undergraduate student
- Scott Ambers, Undergraduate student
- Bill Walsh, Undergraduate student
- Lu Huang, Undergraduate student
- Ben Dennis, Undergraduate student
- Paul Stanfield, Undergraduate student

Collaborations - National

- Vladimir Protopopescu, Oak Ridge National Laborato
- Alan Hunt, Idaho Accelerator Center
- Donald Umstadter, Univesity of Nebraska
- Peter Vanier, Brookhaven National Laboratory
- John Mattingly, Sandia National Laboratories
- Brandon Blackburn, Raytheon
- Andrey Gueorgueiv, Icx Radiation

Collaborations - International

- Imre Pazsit, Andreas Enqvist, Chalmers University of Techn
- Enrico Padovani, Polytechnic of Milan, Italy
- Paul Scoullar, Southern Innovation, Australia
- Peter Schillebeeckx, JRC Geel, Belgium
- Senada Avdic, University of Tusla, Bosnia



Emeritus Faculty

- **Ziya Akcasu**
- **Terry Kammash**
- **Bill Kerr**
- **Glenn Knoll**
- **Dieter Vincent**

Visiting Faculty

Kun-Dar Li, Hsing-Kuo University of Management, Taiwan

Rongsheng Zhou, Shanghai Jiao Tong University, People’s Republic of China

Research Faculty

Mark Hammig, Assistant Research Scientist

Ph.D. (NERS), U of Michigan, 2004

Feng Zhang, Assistant Research Scientist

Ph.D. (NERS), U of Michigan, 2004

Marek Flaska, Assistant Research Scientist

Ph.D. Technical University Delft, The Netherlands, 2006

Zhijie (George) Jiao, Assistant Research Scientist

Ph.D. Polytechnic University New York, 2004

Volkan Seker, Assistant Research Scientist

Ph.D. Purdue University , 2007

Scott Wilderman, Adjunct Research Scientist

Ph.D. (NERS), U of Michigan, 1992

Yunlin Zu, Adjunct Associate Research Scientist

Ph.D. Purdue University , 2004

Adjunct Faculty

Frederick W. Buckman	CEO, Trans-Elect
Mitchell M. Goodsitt	UM Radiology
Randall K. Ten Haken	UM Radiation Oncology
Ruth F. Weiner	Sandia National Lab
Jeremy Busby	Oak Ridge National Lab
John Luginsland	NumerEx (Ithaca, NY)
Forrest Brown	Los Alamos National Lab

Part II. Monte Carlo Methods Development

- Using the chord length distribution functions to compute Dancoff factors
- Coupled deterministic/Monte Carlo methods for VHTR analysis
- “On the fly” Doppler broadening
- Application of the kernel density estimator to fission source convergence and Monte Carlo tallies
- Acceleration of Monte Carlo source convergence
- Functional Monte Carlo for interface effects
- Time-dependent photon transport Monte Carlo

Using the chord length distribution functions to compute Dancoff factors

- **PhD student: Wei Ji (now at RPI)**
- **PhD Advisor: Bill Martin**
- **Collaborator: Forrest Brown**
- **Expected graduation: December 2007**
- **Financial support: DOE NERI DE-FC07-06ID14745**

Summary

- Wei Ji's PhD research was the application of chord length sampling for the analysis of prismatic and pebble bed HTRs
- Derived a chord length PDF starting from assumption of binary stochastic mixture and assuming an exponential distribution
- The mean chord length for an infinite medium can be determined from a simple argument
- The chord length distribution can also be determined empirically
- The chord length distribution function is a powerful quantity and can be used to compute the Dancoff factor for infinite and finite stochastic media

Conventional Dancoff factor

Dancoff factor = average probability a neutron escaping the fuel will enter another fuel region

$$C = \frac{\int dA \int d\Omega \cos\theta (e^{-l/\lambda})}{\int dA \int d\Omega \cos\theta}.$$

Expressed in terms of the chord length pdf

$$C = \int f(l) e^{-l/\lambda} dl.$$

This can be extended to finite region

Convolve the chord length pdf f(l) for the stochastic medium with the chord length pdf F(L) for the finite region (e.g., used to compute Pesc):

$$C^{intra} = \frac{1}{<L>} \int dL F(L) \int_{min\_d}^{L} dl \int_{min\_d}^{l} dl' f(l') e^{-l'/\lambda}.$$

And to a stochastic distribution of finite stochastic regions (eg. Pebble bed)

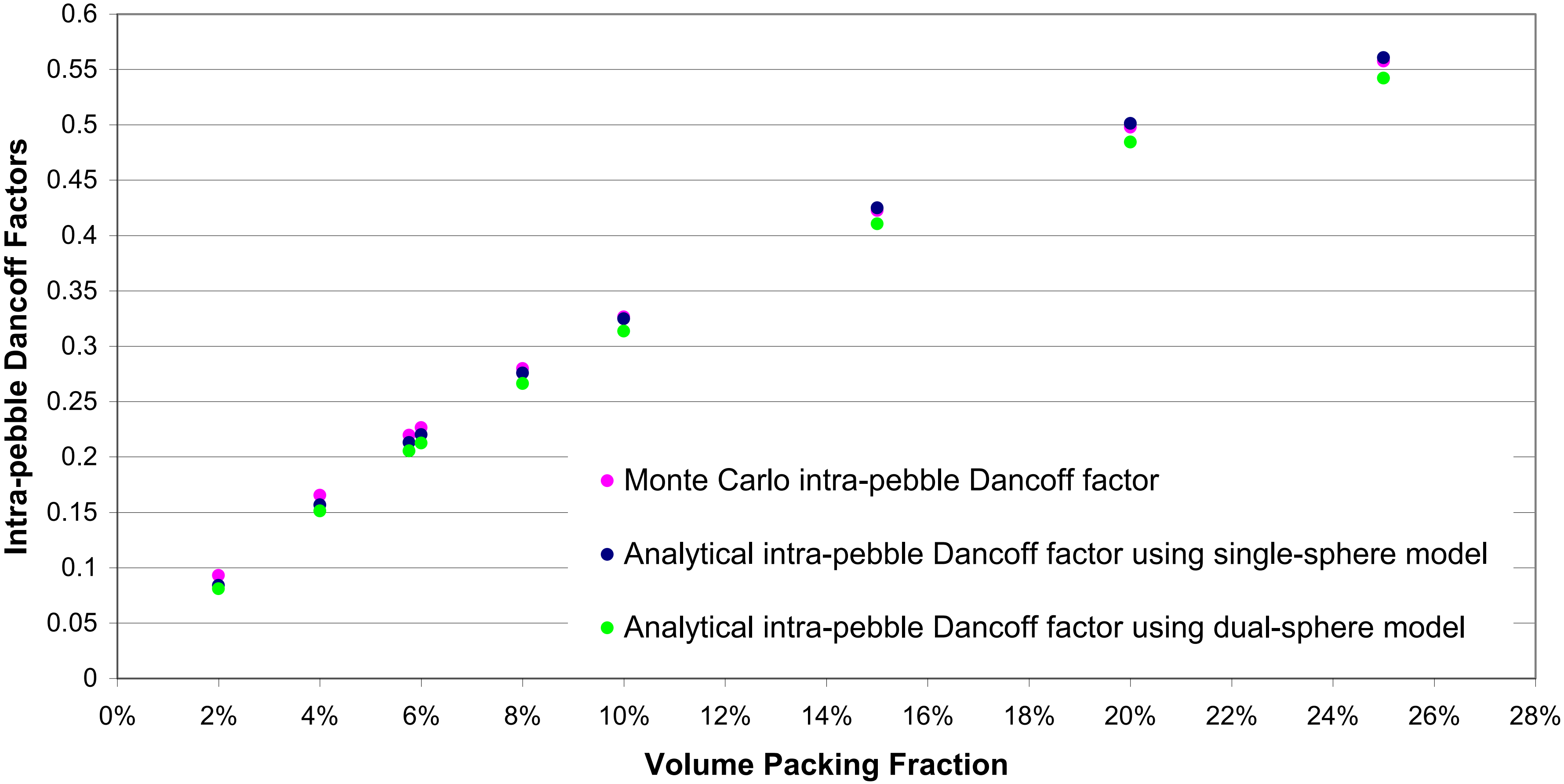
Convolve this with H(S), the chord length pdf between two finite regions:

$$C^{inter} = \frac{\left(\frac{1}{<L>} \int dL F(L) \int_{min\_d}^{L} dl e^{-l/\lambda} \int_{l}^{\infty} f(l')dl' \right) \cdot \left(\int H(S) e^{-S/\lambda} dS \right) \cdot \left(\int dL F(L) \int_{min\_d}^{L} f(l) e^{-l/\lambda} dl \right)}{1 - \left(\int H(S) e^{-S/\lambda} dS \right) \cdot \left(\int dL F(L) e^{-L/\lambda} \int_{L}^{\infty} f(l')dl' \right)}.$$

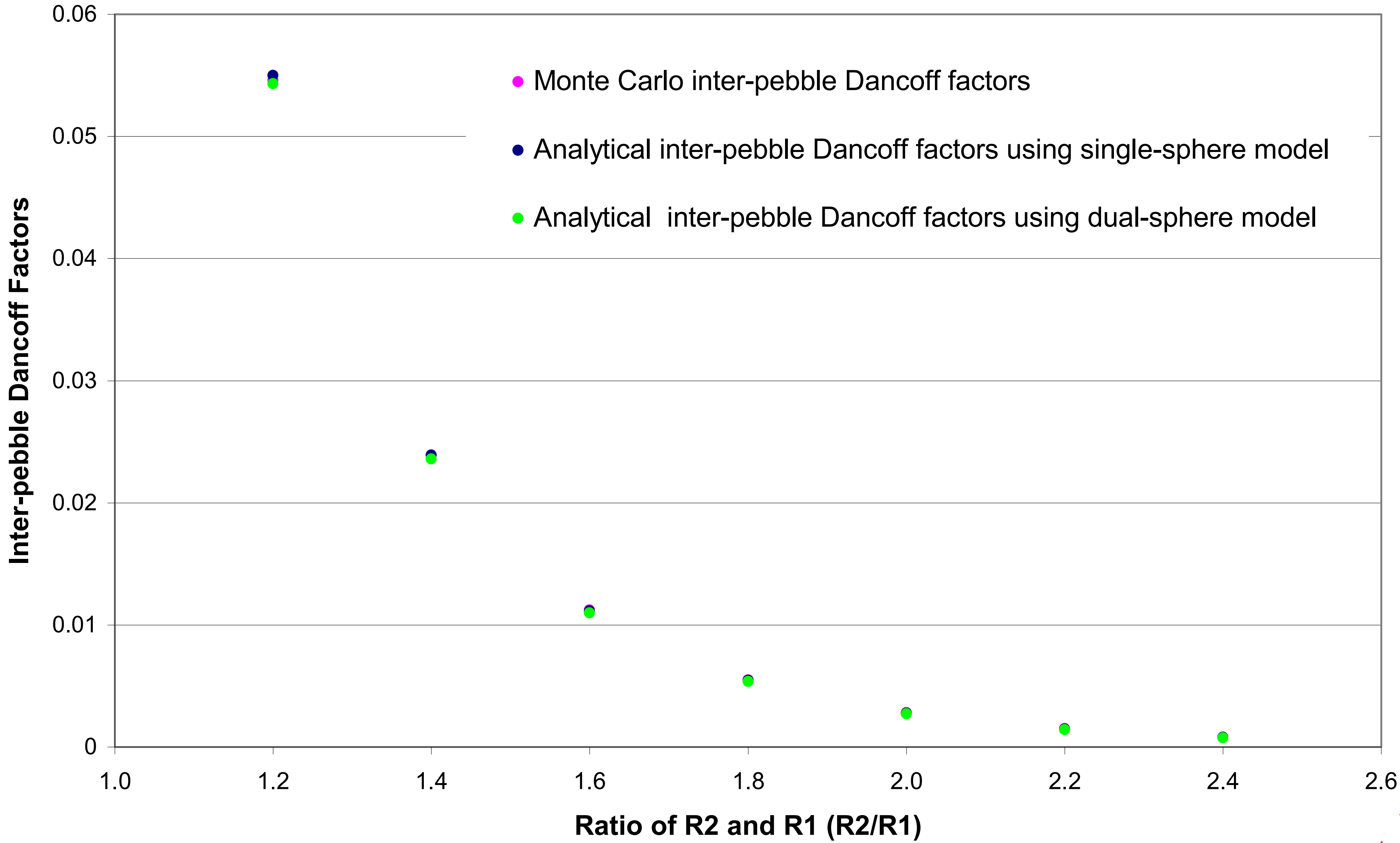
Analytical results with single-sphere model compared to benchmark results

Volume Packing Fractions	Analytical Formula Results $C^{s,\infty}$ Eq.	Benchmark Results C^B (1σ)	Differences $C^{s,\infty}$ - C^B	Relative Error ($C^{s,\infty}$ - C^B)/ C^B
0.0576	0.3515	0.3477 (.0002)	0.0038	1.09%
0.10	0.4857	0.4820 (.0002)	0.0037	0.77%
0.15	0.5873	0.5841 (.0002)	0.0032	0.55%
0.20	0.6559	0.6534 (.0001)	0.0025	0.38%
0.25	0.7054	0.7029 (.0001)	0.0025	0.35%
0.2892	0.7353	0.7331 (.0001)	0.0021	0.30%

Comparison between Analytical and Monte Carlo Intra-pebble Dancoff Factors



Comparisons between analytical and Monte Carlo inter-pebble Dancoff factors at packing fraction 5.76%



Coupled deterministic/Monte Carlo methods for VHTR analysis

- **PhD student: Gokhan Yesilyurt**
- **PhD Advisor: Bill Martin**
- **Collaborator: John Lee**
- **Expected graduation: summer 2009**
- **Financial support: DOE NERI DE-FC07-06ID14745**

Overall Goal and Methodology

- Development, implementation, and testing of a lattice physics code for VHTR neutronic design
- Based on a production LWR lattice physics code augmented by Monte Carlo to treat resonance absorption in TRISO particle fuel.
- MCNP5 computes the resonance absorption rates for specific isotopes in the resonance energy range.
- These are used to compute the fine group resonance group cross sections and they *effectively* overwrite the CPM3 values for these quantities.
- **Earlier version**: CPM-3 and MCNP5 were linked via an Application Program Interface (API), an early deliverable for this study. This path has been set aside.

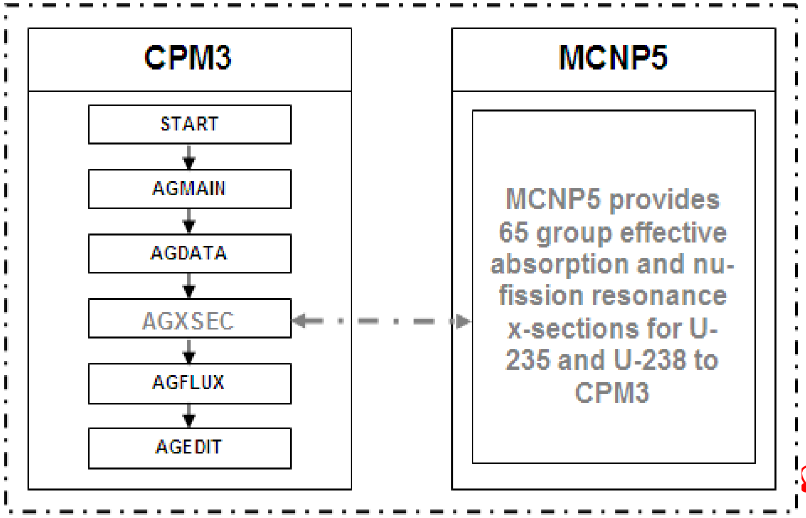
CPM3 and MCNP5 Coupling

- CPM-3 result using standard resonance integral approach with homogeneous fuel:

$$\hat{\sigma}^{i}_{g,res} = \sum_{r \in g} \frac{\hat{I}^{i,r}_{g}}{\Delta u_{g}}$$

- Replace the CPM-3 resonance cross sections by the MCNP5-generated cross sections for all resonance isotopes.

- These adjusted resonance cross sections are then used in the subsequent CPM-3 transport calculation



Alternative – double heterogeneity factor (DHF)

- Define the double heterogeneity factor (DHF):

$$\mathrm{DHF} = \frac{\text{res gp xsec from het MCNP5}}{\text{res gp xsec from hom MCNP5}} = \frac{\sigma_{ag}^{i,\mathrm{MCNP5-het}}}{\sigma_{ag}^{i,\mathrm{MCNP5-hom}}}$$

- The DHF multiplies the CPM-3 resonance xsec
- Assumption: homogeneous MCNP5 yields similar results to CPM3
- <u>Advantages</u>:
  - No need to run MCNP5 and CPM3 simultaneously
  - Allows for full core MCNP5 to compute space-dep DHFs for assemblies in different locations in the core
- The DHF is a self-shielding factor applied to each res group

k_∞

Results for Deep Burn Driver Fuel Compact

Case #	Case Name	k
MCNP5 (Hom)	Homogeneous fuel	1.0408
MCNP5 (Het)	Heterogeneous fuel	1.1043
CPM-3 (Orig)	Original CPM-3	1.0347
CPM-3 (Mod1)	With MCNP5 homogeneous xsecs	1.0391
CPM-3 (Mod2)	With MCNP5 heterogeneous xsecs	1.1038
CPM-3 (Mod3)	With DHFs from hom/het MCNP5 runs	1.1032

k_∞

TRU Fuel Compact

- **Tested the DHF for a realistic TRU fuel composition characteristic of the GA Deep Burn concept.**
- **The fuel kernel consists of Pu-Np-CO representing the Pu-Np isotopics in typical used nuclear fuel (UNF) from light water reactors.**
- **The MCNP5 (homogeneous and heterogeneous fuel) and CPM-3 cases were performed for a fuel compact.**
- **Four different CPM-3 calculations were performed for homogenized driver fuel composition, with different sets of 65 group resonance cross sections.**

Conclusions

- The DHF approach is very attractive. No need to run MCNP5 and CPM3 or Helios simultaneously. This gives flexibility to determine assembly DHFs that depend on spatial location of the assembly in the core because MCNP5 can be run in full core while CPM3 or Helios are run for an assembly.
- We are examining expressing DHFs as a function of Dancoff factors and background cross section to account for their spatial dependence within an assembly or core.
- The DHF methodology has been tested for nominal VHTR fuel assembly and Deep Burn driver fuel compact designs.

"On the fly" Doppler broadening

- PhD student: Gokhan Yesilyurt
- PhD Advisor: Bill Martin
- Collaborator: Forrest Brown
- Expected graduation: summer 2009
- Financial support: DOE NERI DE-FC07-06ID14745

Overall Goal and Methodology

- **Goal**: perform Doppler broadening of the cross sections ***during*** the random walk of neutrons in a Monte Carlo (MC) code.
- **Why**: realistic multiphysics simulations utilizing Monte Carlo for the neutronics module may involve 1000s of material temperatures for which broadened cross sections are needed. Existing Monte Carlo codes (eg, MCNP) were not designed to accommodate this need.
- **Approach**: develop a functional model based on multiple series expansions (Taylor and asymptotic) of the exact resonance model for the cross sections as a function of temperature.
- **Result**: on-the-fly Doppler broadening of the cross sections is possible allowing an unlimited number of temperatures for only a modest computing cost.

Storage and Memory Considerations

Storage space and memory required to perform Monte Carlo simulation with Doppler broadening for full core VHTR and LWR configurations at average fuel centerline temperatures.

MCNP5	$T_{f,ave}$ (K)	Assem-bly Type	# of Assem-blies	Fuel Rods / Assem-bly	Total size of NDF (MB)	Symm-etry	# of Terms in Series Exp.	Total size (MB)
PWR	1000	Square	193	264	132	1/8	-	840,708
VHTR	1300	Prisma-tic	1020	222	129	1/12	-	2,434,230

OTFDC	$T_{f,ave}$ (K)	Assem-bly Type	# Assem-blies	Fuel Rods / Assem-bly	Total size of NDF (MB)	Symm-etry	# of Terms in Series Exp.	Total size (MB)
PWR	1000	Square	-	-	185	-	15	2,775
VHTR	1300	Prisma-tic	-	-	185	-	15	2,775

Theory

- Doppler broadened cross sections for capture and fission can be defined using the psi-chi method:

$$\sigma(E,\xi,x) = \frac{2}{\Gamma_T(E)}\left(\frac{E_R}{E}\right)^{1/2} A(E)\psi(\xi,x)$$

- The simplest and most accurate functional form of $\psi(\xi,x)$:

$$\psi(\xi,x) = \frac{\xi\sqrt{\pi}}{4}\left[exp\left(\frac{(xi-1)^2\xi^2}{4}\right)erfc\left(\frac{\xi - i\xi x}{2}\right) + exp\left(\frac{(xi+1)^2\xi^2}{4}\right)erfc\left(\frac{\xi + i\xi x}{2}\right)\right]$$

$$\xi = \Gamma_T\left(\frac{A}{4kTE_R}\right)^{1/2} \qquad x = 2\frac{(E_r - E_R)}{\Gamma_T}$$

where E_r is the relative energy, E_R is the resonance energy, Γ_T is the total width of the resonance and T is the material temperature.

Theory

- For small values of x (around resonance peak) , Taylor expansion for exp * erfc yields:

$$\sigma(E,T) = \sum_{n=1}^{\infty} \frac{f_n}{T^{n/2}}$$

- For moderate values of x (around the middle of resonance wings), continued fraction expansion for exp * erfc yields:

$$\sigma(E,T) = \sum_{n=1}^{\infty} g_n T^{n/2}$$

- For high values of x (low end of resonance wings) , asymptotic expansion for exp * erfc yields:

$$\sigma(E,T) = \sum_{n=0}^{\infty} h_n T^n$$

Theory

- **Objective**: our functional model for a given nuclide should cover the following range of temperatures:

Temperature Range	Field of Study
77K - 293.6K	Cold Neutron Physics
293.6K - 550K	Benchmarking Calculations
550K - 1600K	Reactor Operation
1600K - 3200K	Accident Conditions

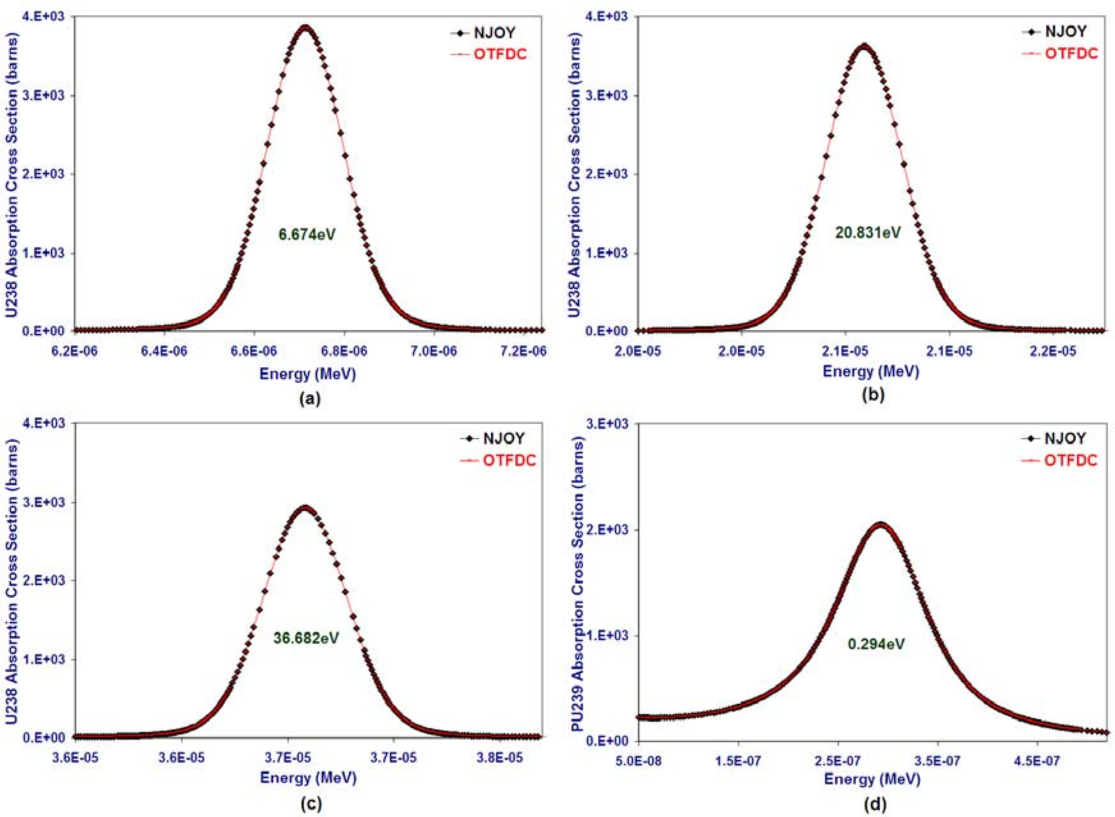
- **Result**: the following functional form represents the best fit of cross sections for this energy range:

$$\sigma(E,T) = \sum_{n=1}^{7} \frac{f_n}{T^{n/2}} + c + \sum_{n=1}^{7} g_n T^{n/2}$$

Discretization of Doppler Broadening Kernel

- A several times faster version (OTFDC) of the well-known Doppler broadening kernel developed by Cullen was implemented in C++ :

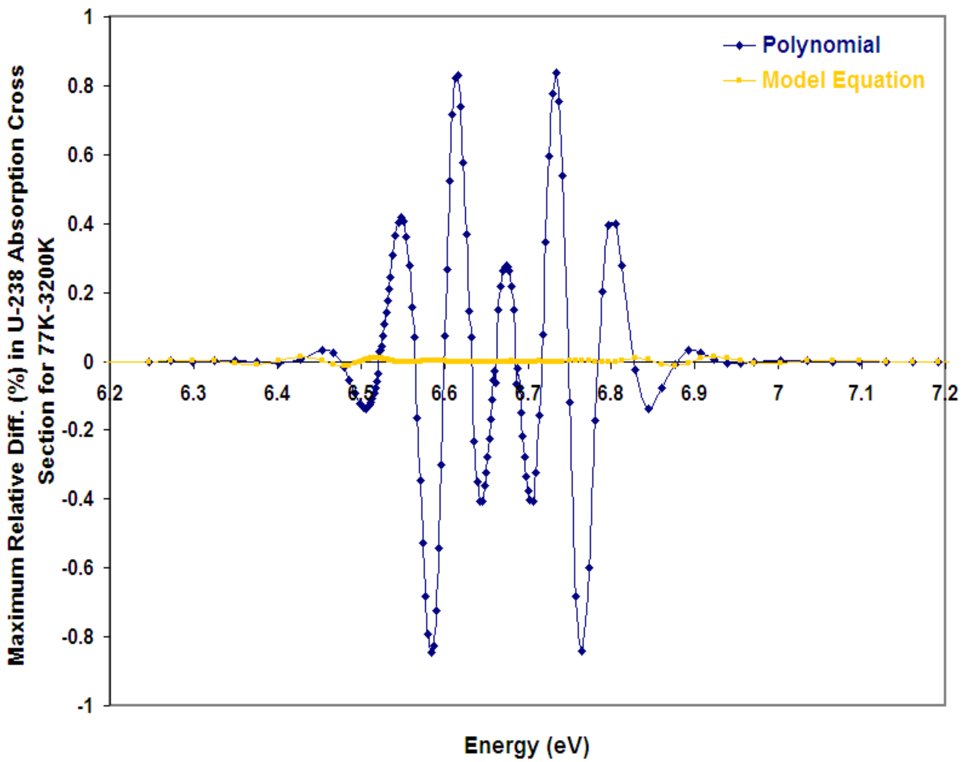
$$\sigma(y,T_2)=\frac{1}{y^2}\left(\frac{1}{\pi}\right)^{\frac{1}{2}}\int_0^\infty \sigma(x,T_1)x^2\left[e^{-(x-y)^2}-e^{-(x+y)^2}\right]dx$$

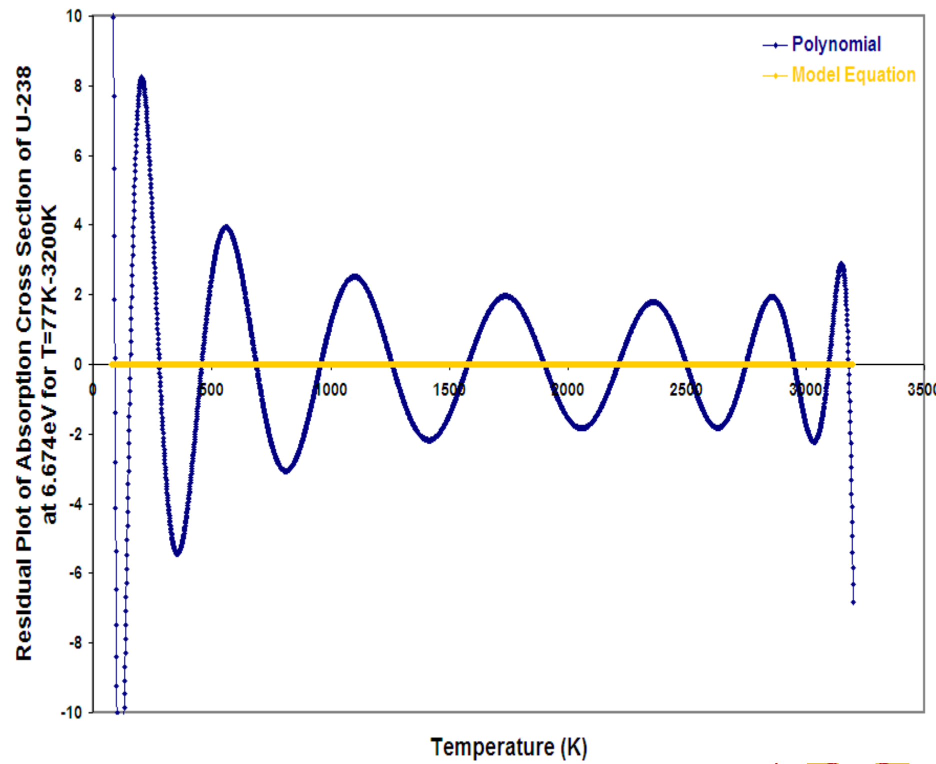


It was found that the maximum difference in cross sections over the entire energy grid points for all important resonance absorber nuclides is less than 1e-5% between NJOY and OTFDC at T=1300K.

Some Results

- OTFDC was used to generate cross sections between 77K-3200K for a given energy point between 77K and 3200K. Data fit to our model equation is excellent.





Timing Results

- A Monte Carlo transport code was written for timing the Doppler broadening methodology.

- The free gas thermal model was applied to sample the motion of the target atom in the medium. The conventional pdf for target velocity and collision angle were used.

- It was found that model equation can be used in Monte Carlo codes to Doppler broaden the cross sections on-the-fly with a computing cost less than 1% with discarding the cross section after it used and allowing an unlimited number of temperatures.

Application of the kernel density estimator to fission source convergence and Monte Carlo tallies

- **PhD student: Kaushik Banerjee**
- **PhD Advisor: Bill Martin**
- **Expected graduation: summer 2009**
- **Financial support: DOE NERI DE-FC07-06ID14745 and DOE NEER DE-FG07-04ID14607**

Kernel Density Estimator Methods

- Kernel Density Estimator (KDE), a non-parametric probability density estimator, is used to estimate MC scalar flux tallies.
- KDE tally can entirely eliminate the requirement of bin structure.
- KDE tally can be used to estimate flux at a point.
- KDE tally performance is better than point detector tally when the detector point is placed in a source/scattering region.

KDE Collision and Track-length tally

- Collision tally

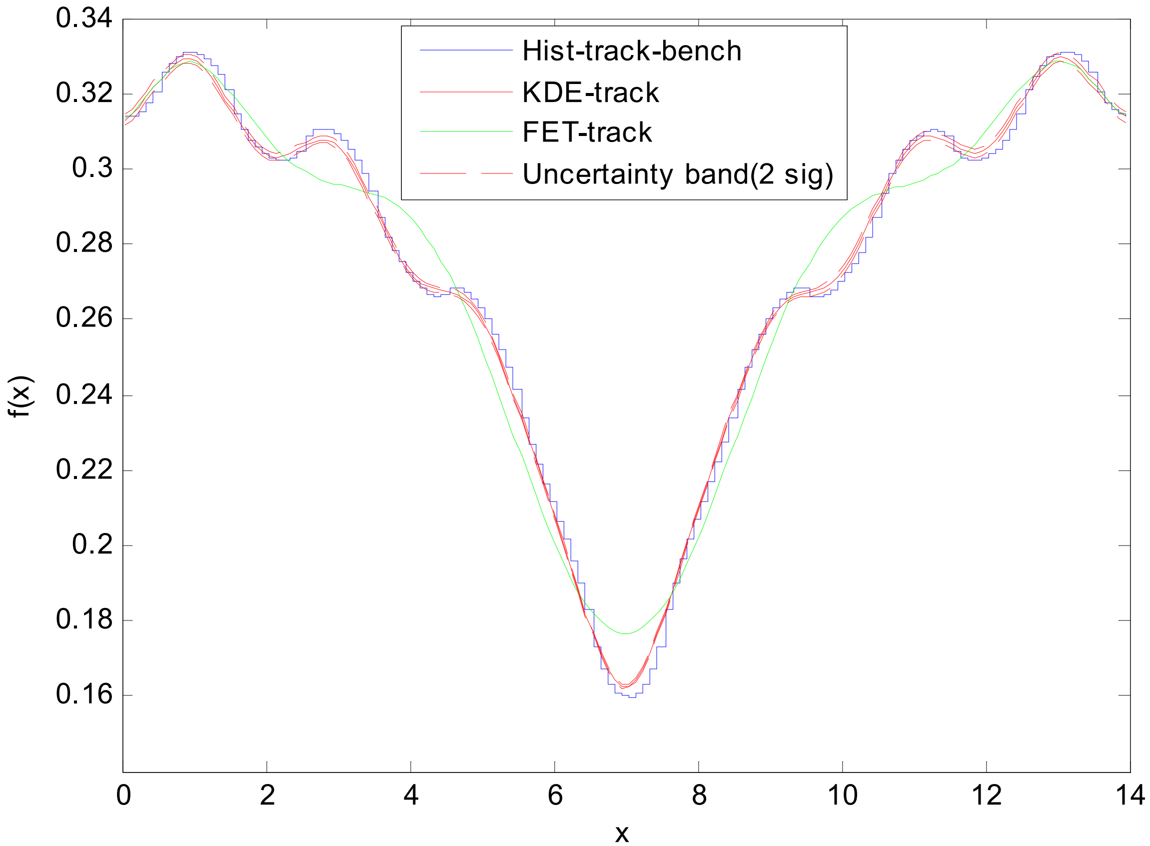
$$\Phi(x) = \frac{1}{N}\sum_{i=1}^{N}\sum_{c=1}^{C_i}\frac{w_{i,c}}{\Sigma_t(X_{i,c})}\frac{1}{h}k\left(\frac{x - X_{i,c}}{h}\right)$$

- Track-length tally

$$\Phi(x) = \frac{1}{N}\sum_{i=1}^{N}\sum_{c=1}^{C_i}\frac{w_{i,c}d_{i,c}}{n}\sum_{j=1}^{n}\frac{1}{h}k\left(\frac{x - X_{i,c,j}}{h}\right)$$

- k(x) is the kernel function which can be any positive probability density function.

KDE tally numerical example



For Histogram
10^5 particles/cycle
300 total cycles
100 discarded

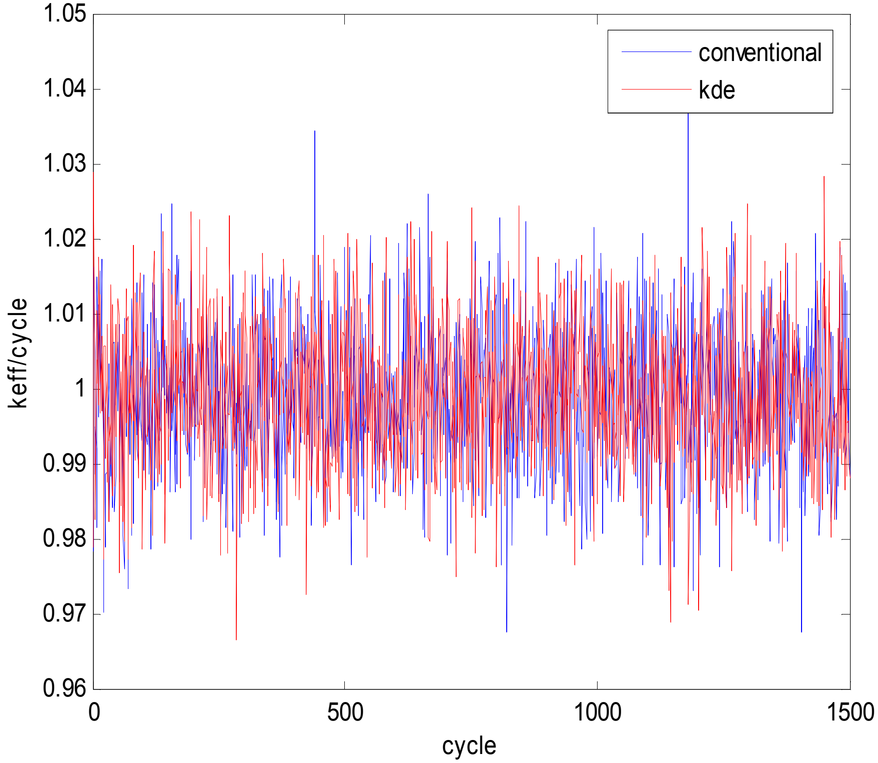
For KDE and FET
2 x 10^4 particles/cycle
150 total cycles
50 discarded
n = 4

One group flux distribution inside a 1D array of fuel and water with a strong neutron absorber in the center by track length estimator.

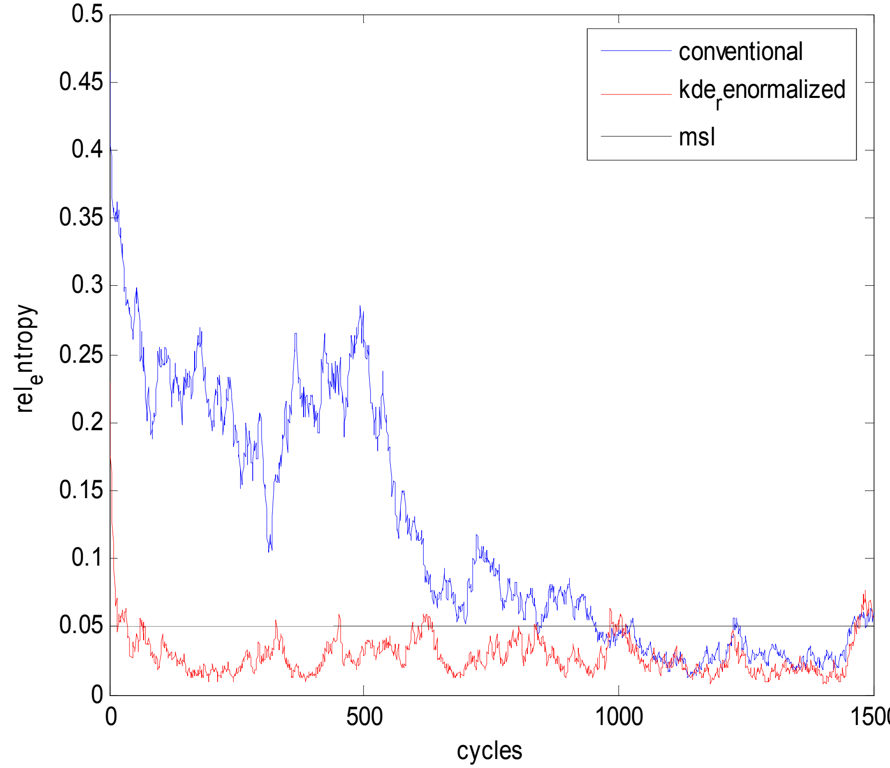
KDE fission source sampling

- KDE is also used to accelerate fission source convergence for loosely coupled systems.
- At the end of each cycle KDE is used to estimate the fission source distribution.
- Fission sites for the next generation are sampled from the estimated distribution.
- Sampling is on-the-fly, no need to construct the whole fission distribution.

KDE fission source numerical example – 1D slab geometry(100 mfp)



Cyclewise Keff for conventional and KDE method.



Posterior relative entropy comparison between conventional and KDE

10,000 particles/batch, 1500 batches, 500 skipped

Acceleration of Monte Carlo source convergence

- **PhD student: Bryan Toth**
- **PhD Advisor: Bill Martin**
- **Collaborators: James Holloway and Dave Griesheimer (Bettis)**
- **Expected graduation: summer 2009**
- **Financial support: Naval Reactors Rickover Fellowship**

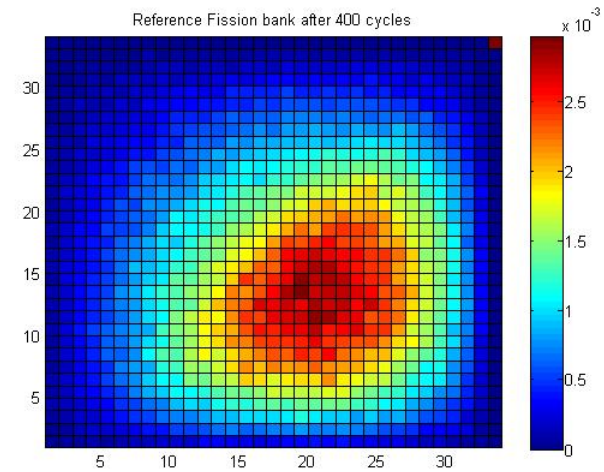
Source Convergence Acceleration

- Extrapolate fission source $u^{(m)}(R)$ at cycle *m* using the change from an application of the transport operator $k^{-1}A$

$$u^{(m+1)}(R) = k^{-1}Au^{(m)}(R) + \alpha\left(k^{-1}Au^{(m)}(R) - u^{(m)}(R)\right) \quad (1)$$

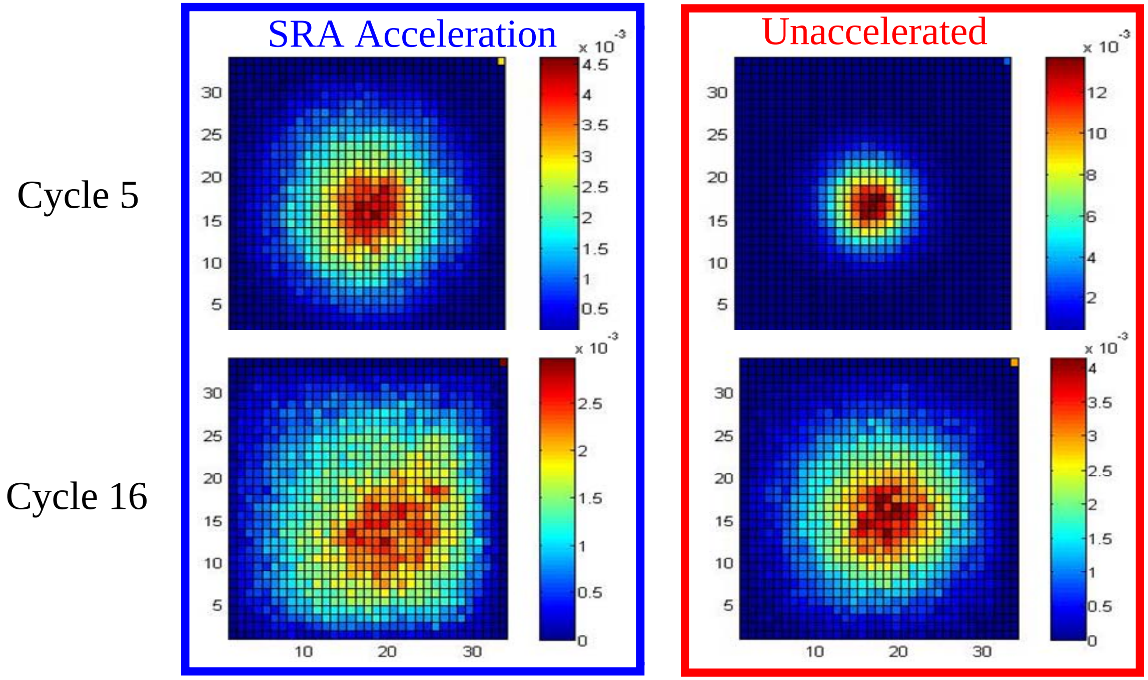
- Compute the difference in Eq. (1) on a coarse mesh to filter out high frequency modes
- Select more or less fission sites from within a mesh box based on the computed difference
- The acceleration is stopped prior to starting active cycles
- This method has minimal computational overhead

Source Convergence Acceleration Results



Reference Solution

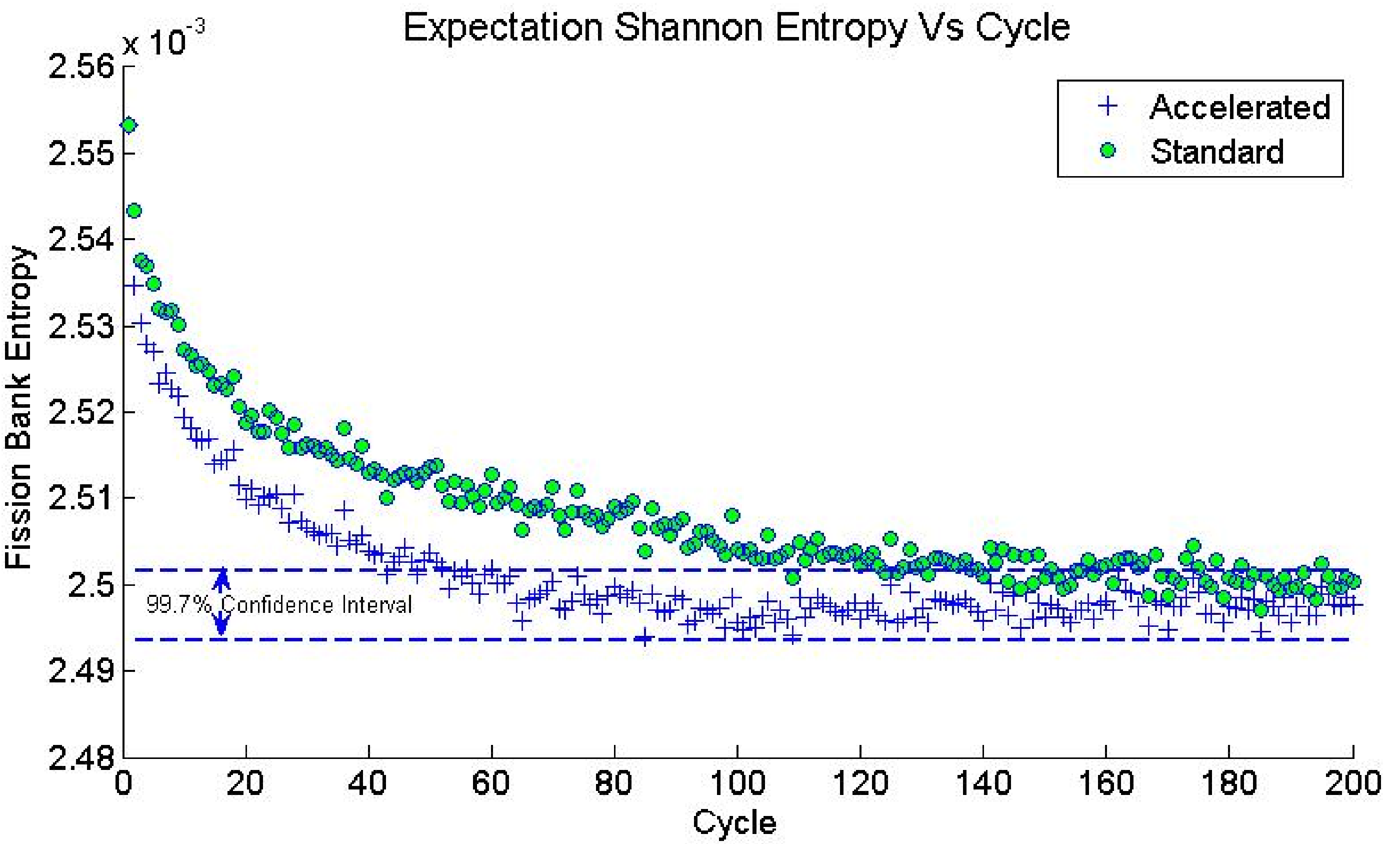
Converged source distribution of a 2-D simplified reactor problem, represented as a 32×32 histogram. Solution was calculated using 400 cycles, with 400,000 neutrons per cycle, starting from an initial point source.



Fission source distributions for the 2-D simplified reactor model after 5 and 16 cycles, using Monte Carlo with (blue box) and without (red box) source acceleration. All source distributions are represented as a 32×32 histogram. Solutions were calculated using 160,000 neutrons per cycle, starting from an initial point source. One can see that the accelerated simulation is significantly closer to the reference solution than the standard simulation at both ot the displayed cycles.

Source Convergence Acceleration Results

Observed discard cycle savings exceeds 100 cycles, a 50% reduction for a uniform 60 mean free paths thick slab with a flat starting source.



Source Convergence Acceleration Future Work

- Determine optimal extrapolation parameter α which depends on problem geometry and mesh size
- Develop an on-the-fly diagnostic to determine the cutoff cycle
- Investigate eigenvector frequency spectrum to dictate optimal filtering technique

Functional Monte Carlo for interface effects

- PhD student: Emily Wolters
- PhD Co-advisors: Bill Martin and Ed Larsen
- Expected graduation: 2010
- Financial support: DOE NE Fellowship

Overview

- Hybrid (Monte Carlo-deterministic) method
- Analysis of problems with interface transport effects (e.g. group fluxes strongly dependent on angle)
- Conventional deterministic methods (multigroup S_N) fail to preserve these effects because of the multigroup approximation which assumes an isotropic flux weighting function
    - Incorrect reaction rates and eigenvalues unless # of energy groups very large (for simplified ABR in ANL analysis, G>300)

Derivation of functional method

- Avoids multigroup approximation by defining angle dependent "functionals", computed by Monte Carlo
- Functionals defined by applying $\pm\int_0^{\pm 1} d\mu \int_0^{\infty} dE$ to transport equation (1D fixed source problem for now) and then applying a spatial mesh
- Resulting functionals look like

$$\Sigma_{i,j}^{\pm} \equiv \frac{\pm\int_{x_{j-1/2}}^{x_{j+1/2}} dx \int_0^{\infty} dE \int_0^{\pm 1} d\mu \Sigma_i\left(x,E\right)\psi\left(x,\mu,E\right)}{\pm\int_{x_{j-1/2}}^{x_{j+1/2}} dx \int_0^{\infty} dE \int_0^{\pm 1} d\mu\, f\left(x,E\right)\psi\left(x,\mu,E\right)}$$

$$\mu_{j+1/2}^{\pm} \equiv \frac{\pm\int_0^{\infty} dE \int_0^{\pm 1} d\mu \mu\psi\left(x_{j+1/2},\mu,E\right)}{\pm\int_0^{\infty} dE \int_0^{\pm 1} d\mu\, f\left(x_{j+1/2},E\right)\psi\left(x_{j+1/2},\mu,E\right)}$$

- f(x,E) is the desired reaction cross section (or 1 for scalar flux)

High and Low Order Equations

- Computation of functionals by Monte Carlo
  - Model the exact problem in Monte Carlo and tally the quantities in the numerators and denominators of the functionals
  - Since the functionals are ratios of flux tallies, they have less variance than the flux tallies themselves (standard Monte Carlo)
- Using the functionals to solve the problem
  - Defining the functionals this way leads to a system of low-order eqns easily solved with modified one group discrete ordinates theory

$$\frac{1}{\Delta x_j}\left[\mu^+_{j+1/2}F^+_{j+1/2} - \mu^+_{j-1/2}F^+_{j-1/2}\right] + \frac{\Sigma^+_{t,j}}{2}\left(F^+_{j+1/2} + F^+_{j-1/2}\right) = S^+_j$$

$$\frac{1}{\Delta x_j}\left[\mu^-_{j+1/2}F^-_{j+1/2} - \mu^-_{j-1/2}F^-_{j-1/2}\right] + \frac{\Sigma^-_{t,j}}{2}\left(F^-_{j+1/2} + F^-_{j-1/2}\right) = S^-_j$$

Preliminary Results

- Preliminary Test Problem
  - Geometry: Slab “core” surrounded by “reflector” (artificial materials)
  - Source: Fixed volumetric, 0.9-1 MeV, isotropic source in “core”
  - Desired Quantity: Capture rate distribution
- Results
  - Solution agreed with benchmark M.C.
  - Variance less than standard M.C. (Figure of Merit twice as high)
- Future work
  - Working on a more complicated problem to show improvement over conventional deterministic methods
  - Extension of method to incorporate more general scattering, eigenvalue problems, and more complex geometry

Conclusions and Next Steps

- Recap of Advantages
  - Anticipated to capture transport effects better than conventional deterministic methods
  - Faster than standard Monte Carlo
  - Eliminates user intuition decisions such as group boundaries and number of discrete ordinate directions; no cross-section collapsing
  - Possible application to ray effect problems
- Next conference presentation
  - Mathematics & Computation Conference in Saratoga Springs, NY (May, 2009)

Time-dependent photon transport Monte Carlo

- **PhD student: Jesse Cheatham**
- **PhD Co-advisors: Bill Martin and James Holloway**
- **Expected graduation: Summer 2009**
- **Financial support: DOE NEER DE-FG07-04ID14607 and ASC PSAAP Center Grant (CRASH - Center for Radiative Shock Hydrodynamics)**

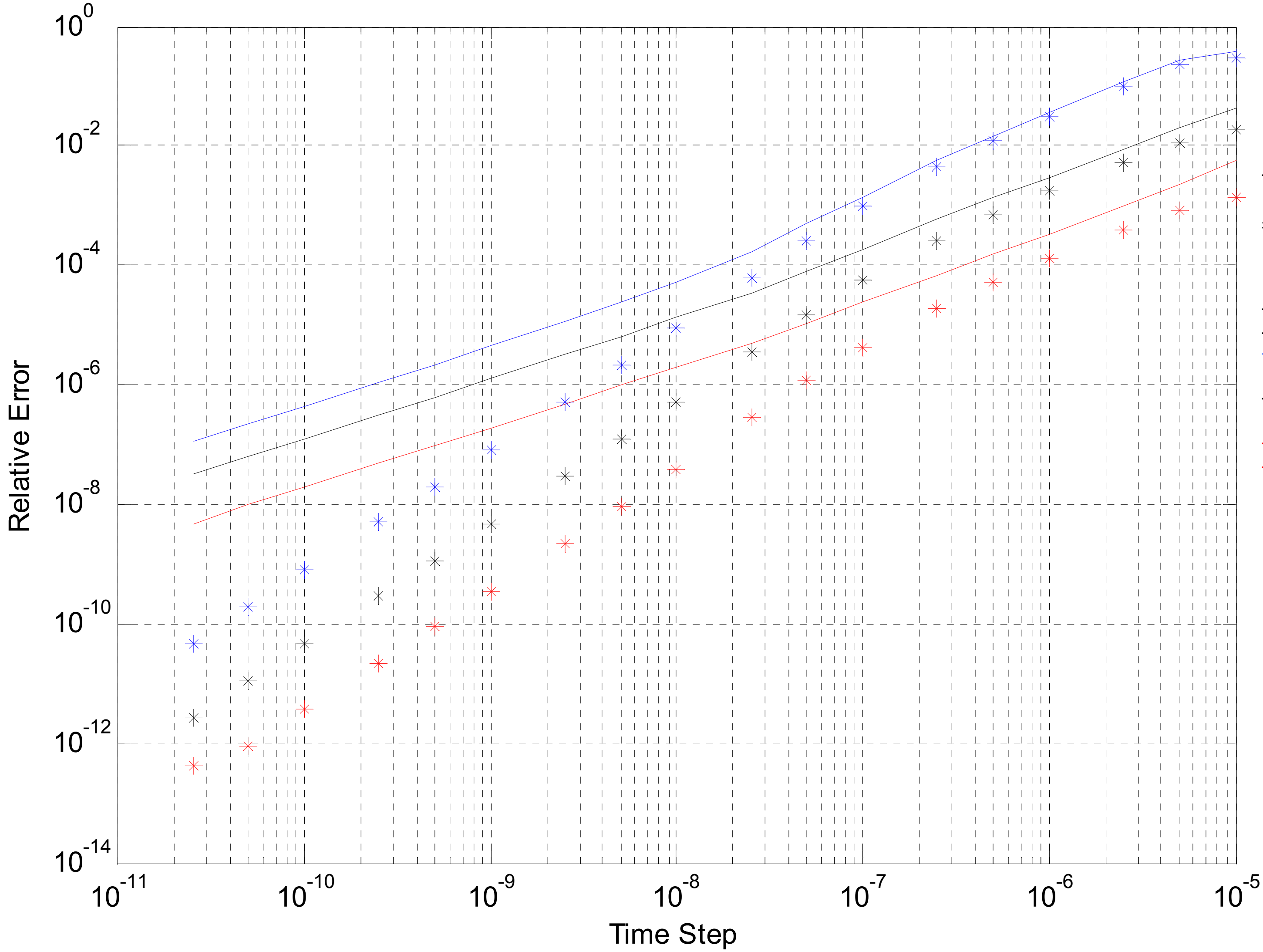
Thermal Radiative Transfer Equations

- **1971: Implicit Monte Carlo (IMC) Method proposed by Fleck and Cummings**
  - Assumes functional form of the emissivity
  - Assumes all absorptions have instantaneous emission
- **1973: Carter and Forest (CF) propose more exact treatment of physics**
  - Computationally more intensive (use of exponentials for time delayed emissions and scattering)
  - Both CF and IMC first order accurate
  - No practical gain seen with more accurate physics for realistic problems- CF never got traction at the labs

Predictor-Corrector Methods

- A detailed truncation error analysis demonstrates the opacity is the dominant source of error
- Predictor step uses traditional IMC or CF then the Corrector step changes the opacity depending on the temperature at the end of the Predictor step
- The Carter-Forest method is dominated by the approximation to the opacity, while IMC is dominated by the opacity estimation and the approximate functional form of the emissivity
  - Result: CF becomes 2nd order while IMC is still 1st order in time

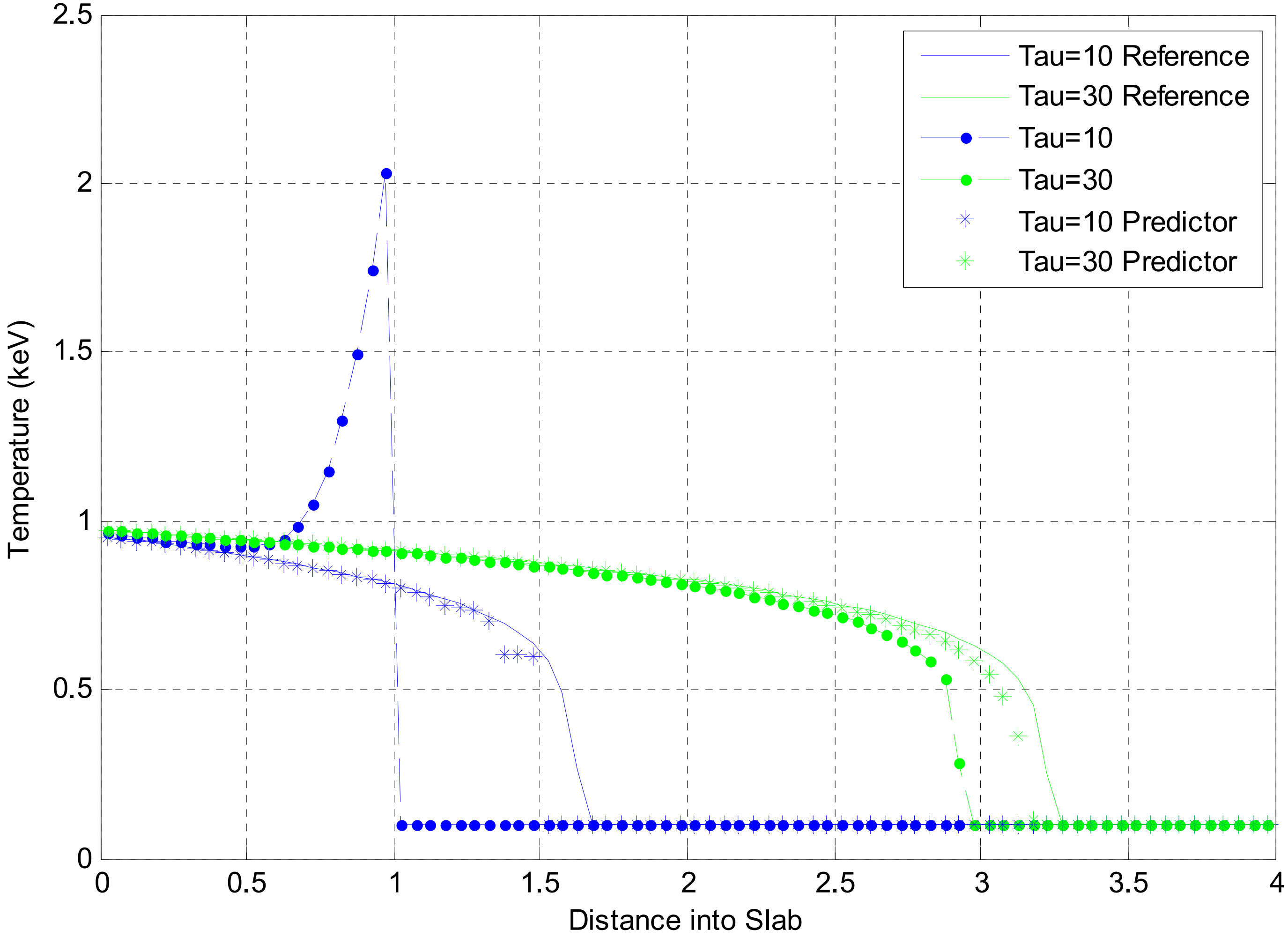
Relative Error of a Deterministic Predictor-Corrector IMC and CF Compared with a Reference Solution



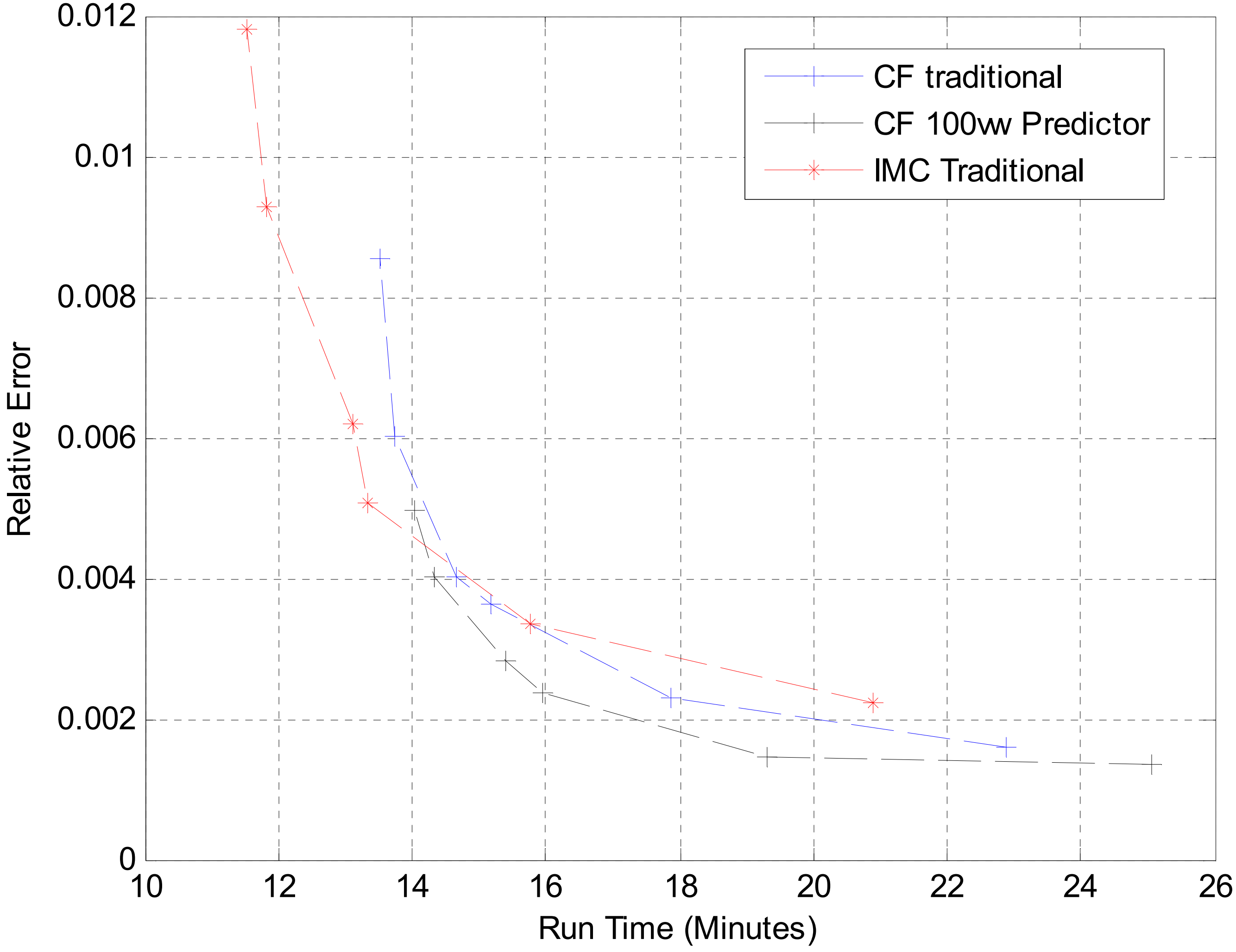
Lines = IMC
*** = CF**

In seconds
Blue = 10^-5
Black =5*10^-5
Red = 10^-4

1D Marshak Wave
dx=0.05 dTau=0.01 dTau(ref)=0.05
(Standard vs. Pred-Corr)



1D Relative Error using the time step sizes of 0.1, 0.08, 0.05, 0.04, 0.02, 0.01



100w: 100x more particles for corrector step than for predictor step