# CCS-4 Publications and Other Performance Indicators
# March 2005 to March 2006

## CCS-4 Peer-Reviewed Journal Publications

A. Socrates, O. Blaes, A.L. Hungerford, C. Fryer, "The neutrino bubble instability: a mechanism for generating pulsar kicks," The Astrophysical Journal, 632, 531, 2005.

A.L. Hungerford, C. Fryer, G. Rockefeller, "Gamma-Rays from Single-Lobe Supernova Explosions," The Astrophysical Journal, 635, 487, 2005.

A.L. Hungerford, C. Fryer, F. Timmes, K. McGhee, "Nucleosynthetic Signatures of Asymmetric Supernovae - Lessons Learned from 1-dimensional simulations," Nuclear Physics A, 758, 15, 2005.

C. Fryer, A.L. Hungerford, F. Timmes, "Changing the r-Process Paradigm," Nuclear Physics A, 758, 599, 2005.

C. Kulesa, A.L. Hungerford, C. Walker, X. Zhang, A. Lane, "Large-Scale CO and [CI] Emission in the rho Ophiuchi Molecular Cloud," The Astrophysical Journal, 625, 194, 2005.

J.D. Densmore, "Interface Methods for Hybrid Monte Carlo-Diffusion Radiation-Transport Simulations," Ann. Nucl. Energy, 33, 343, 2006.

J.E. Morel, B. B.T. Adams, J.M. McGhee, T.M. Evans, T.J. Urbatsch, "Spatial Discretizations for Self-Adjoint Forms of the Radiative Transfer Equations," Journal of Computational Physics, v.214, p.12-40, 2006.

J.E. Morel, J.S. Warsa, "An SN Spatial Discretization Scheme for Tetrahedral Meshes," Nuclear Science and Engineering, v. 151, pp. 157-166, 2005.

R.C.Ward, R.S.Baker, J.E.Morel, "A Diffusion Synthetic Acceleration Method for Block Adaptive Mesh Refinement," Nuclear Science and Engineering, 152, 164-179, 2006. LA-UR-05-1968.

T.A. Brunner, T.J. Urbatsch, T.M. Evans, N.A. Gentile, "Comparison of Four Parallel Algorithms for Domain Decomposed Implicit Monte Carlo," Journal of Computational Physics, Mar 1 2005; v.212, no.2, p.527-539. SAND-2004-6694J; LA-UR-05-0290, UCRL-JRNL-208745.

## CCS-4 Book Chapters

D. Carrington, D. Pepper, Indoor Air Pollution Modeling, Chapter 14 of Air Quality Modeling, Theories, Methodologies, Computational Techniques, Available Databases and Software, Vol. II Advanced Topics, Zannetti, P. (editor). Also a technical report, LA-UR-04-2508, Los Alamos National Laboratory. 2005.


## CCS-4 Papers Published in Conference Proceedings

D.B. Carrington, S.A. Turner, "Explicit Correction for Material Motion in Radiative Transport (U)," LA-UR-05-3789, May 2005. Proceedings for Five Lab Conference in Vienna, Austria, June 19-24, 2005. The five labs were LANL, LLNL, SNL, VNIIEF, and VNIITF.

J.A. Dahl, "3-D Extension C5G7 MOX Benchmark Results Using PARTISN," LA-UR-05-0289, International Topical Meeting on Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, September 12-15, 2005.

J.D. Densmore, T.J. Urbatsch, T.M. Evans, M.W. Buksas, "Discrete Diffusion Monte Carlo for Grey Implicit Monte Carlo Simulations," Proc. International Topical Meeting on Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, September 12-15, 2005.

J.E. Morel, A. Gonzalez-Aller, J.S. Warsa, "A Lumped Discontinuous Finite-Element Spatial Discretization for Triangular-Mesh SN Calculations in R-Z Geometry," Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, Sept. 12-15 2005.

J.E. Morel, J.S. Warsa, "SN Finite Element Lumping on Quadrilateral Meshes in X-Y Geometry," Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, Sept. 12-15 2005.

J.H. Chang, M.L. Adams, "Effectiveness of Various Transport Synthetic Acceleration Methods With and Without GMRES," Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, Sept. 12-15 2005. LA-UR-05-0326.

J.S. Warsa, K.G. Thompson, J.E. Morel, J.H. Chang, K.G. Budge, M. Benzi, "Preconditioning a Parallel, Inexact Block-Jacobi Splitting of the SN Algorithm," included in the conference proceedings of the International Topical Meeting on Mathematics and Computation, Super Computing, Reactor Physics, and Nuclear Biological Applications, 2005 September 12-15, Avignon, France. LA-UR-05-1097, LA-UR-05-2256.

J.S. Warsa, K.G. Thompson, J.E. Morel, J.H. Chang, K.G. Budge, M. Benzi, "Preconditioning a Parallel, Inexact Block-Jacobi Splitting of the SN Algorithm,"

included in the conference proceedings of the 2005 International Conference On Preconditioning Techniques For Large Sparse Matrix Problems In Scientific And Industrial Applications, 2005 May 19-21, Emory University, Atlanta, Georgia. LA-UR-05-0728.

R.C. Ward, R.S. Baker, J.E. Morel, "A Diffusion Synthetic Acceleration Method for Block Adaptive Mesh Refinement," Intl. Mtg. on Mathematics and Computation., Supercomputing, Reactor Physics, and Nuclear and Biological Applications, Avignon, France September 12-15, 2005. LA-UR-05-4684.

S.W. Mosher, F. Rahnema, "A Decoupled Finite Element Heterogeneous Coarse Mesh Transport Method," Trans. Am. Nucl. Soc., v. 92, 2005. LA-UR-05-0696.

S.W. Mosher, J.D. Densmore, "Stability and Monotonicity Conditions for Linear, Grey, 0-D Implicit Monte Carlo Calculations," Trans. Am. Nucl. Soc. v. 93, 520, 2005. LA-UR-05-4780.

T.A. Brunner, T.J. Urbatsch, T.M. Evans, N.A. Gentile. "Comparison of Four Parallel Algorithms for Domain Decomposed Implicit Monte Carlo," Mathematics and Computation, Supercomputing, Reactor Physics, and Nuclear and Biological Applications, September 12-15, 2005. American Nuclear Society. Avignon, France.


## CCS-4 Invited Presentations at Professional Meetings

A.L. Hungerford, "Gamma-Ray Emission from Asymmetric Supernovae," Institute for Pure and Applied Mathematics: Supernova Focus Day, Los Angeles, CA, April 2005.

A.L. Hungerford, "Monte Carlo Simulations of Neutrino Heating in Neutron Stars," Physics and Astrophysics of Supernova Neutrinos, Santa Fe, NM, July 18-22, 2005.

A.L. Hungerford, "Nucleosynthesis in Asymmetric Supernovae," Supernova and Gamma-Ray Burst Remnants, Santa Barbara, CA, February 2006.

J.D. Densmore, T.J. Urbatsch, T.M. Evans, M.W. Buksas, "A Hybrid Transport-Diffusion Method for Monte Carlo Radiative Transfer Simulations," Five-Laboratory Conf. on Computational Mathematics, Vienna, Austria, June 19-23, 2005. LA-UR-05-3901.

J.D. Densmore, "Discrete Diffusion Monte Carlo for Grey Implicit Monte Carlo Simulations," Physics and Astrophysics of Supernova Neutrinos, Santa Fe, NM, July 18-22, 2005.

J.S. Warsa, "Krylov Methods for Radiation Transport Calculations," presented at the IPAM Grand Challenge Problems in Computational Astrophysics Workshop IV: Transport Phenomena, 16-20 May 2005, UCLA, Los Angeles, CA. LA-UR-05-3609.

J.S. Warsa, J.E. Morel, "Full Lumping of the Quadrilateral Mesh Discontinuous Finite Element Sn Transport Equations in r-z Geometry," presented at the LACSI Symposium 2005, Workshop on Advanced Numerical Methods for PDEs, 11-13 Oct 2005, Santa Fe, NM. LA-UR-05-7970.

K.G. Budge, "Astrophysical Neutrino Transport with Capsaicin," Physics and Astrophysics of Supernova Neutrinos, Santa Fe, NM, July 18-22, 2005 LA-UR-05-5374.

T.J. Urbatsch, "Some Radiation Transport Methods and Research Potentially Applicable to Neutrino Simulations," Physics and Astrophysics of Supernova Neutrinos, Santa Fe, NM, July 18-22, 2005.


## CCS-4 Unclassified Reports

A.L. Hungerford, J.D. Densmore, M.W. Buksas, "Compton Scattering in Implicit Monte Carlo(U)," CCS-4:05-14, 2005.

J.A. Dahl, "PARTISN Results for the OECD/NEA 3-D Extension C5G7 MOX Benchmark," LA-UR-05-6281.

J.A. Dahl, "Software Requirements Specification for Group Dependent Restarts(U)," CCS-4:05-49, LA-UR-05-6723, Los Alamos National Laboratory, August 29, 2005.

J.D. Densmore, M.W. Buksas, T.M. Evans, Todd Urbatsch, "Release of ClubIMC-2_0_0(U)," CCS-4:05-07, January 19, 2005.

J.D. Densmore, A.L. Hungerford, T.J. Urbatsch, T.M. Evans, "Vision and Scope Statements for Project Eazy-E(U)," CCS-4:05-08, January 20, 2005.

J.D. Densmore, D.B. Carrington, "Emissivity of Discretized Diffusion Problems(U)," CCS-4:05-23 (LA-UR-05-3249), April 25, 2005.

J.D. Densmore, T.M. Evans, A.L. Hungerford, "A Semi-Implicit Treatment of Compton Scattering in Implicit Monte Carlo Simulations (U)," CCS-4:05-57, October 19, 2005.

J.D. Densmore, T.M. Evans, "Discrete Diffusion Monte Carlo for XY AMR Meshes, CCS-4:06-04, February 15, 2006.

J.E. Morel, J.S. Warsa, "Spatial Finite-Element Lumping Techniques for the Quadrilateral Mesh Sn Equations in X-Y Geometry," LA-UR-06-0715.

J.D. Edwards, "Summary of 2005 GRA research activities: Comparison of Lumped and Unlumped DFEMs for Solving the Neutron Transport Equation." LA-UR-05-6372.

K.G. Thompson, "Problem set for the Q2FY05 Capsaicin L2 ASC milestone review," Los Alamos National Laboratory, Memorandum, CCS-4:05-01(U), Jan., 2005.

K.G. Thompson, "An Update of the Capsaicin Q2FY05 ASC Milestone Statement, Revision 3," Los Alamos National Laboratory, Research Note, CCS-4:05-02(U), Jan., 2005.

K.G. Thompson, K.G. Budge, J.S. Warsa, J.H. Chang, "Release of Capsaicin-2_2_2," Technical Memorandum, 2005 March 4. LA-UR-05-2256.

K.G. Thompson, K.G. Budge, J.S. Warsa, J.H. Chang, "Completion of Deterministic Radiative Transfer Simulation ASC Level 2 Milestone," Technical Memorandum, 2005 March 29. LA-UR-05-2287.

K.G. Thompson, "The Capsaicin Project: A status report following the completion of the Q2FY05 LANL L2 milestone," Presentation, 2005 April 29. LA-UR-05-3235.

K.G. Thompson, K.G. Budge, J.H. Chang, A. Gonzalez-Aller, J.S. Warsa, "Transport Methods Research Results from the Capsaicin Project," Presented at the Computer and Computational Sciences Division Review, 2005 May 31 - June 2. LA-UR-05-3915.

K.G. Thompson, "Release of Capsaicin-2_5_0," Los Alamos National Laboratory, Memorandum, CCS-4:05-44(U), August, 2005.

K.G. Thompson, "Compilers and Options Recommended by the Capsaicin Team," Los Alamos National Laboratory, Memorandum, CCS-4:05-69(U), November, 2005.

K.G. Thompson, "Summary of Q1FY06 WSR Activities for the Capsaicin Team," Los Alamos National Laboratory, Memorandum, CCS-4:06-01(U), January, 2006.

R.C.Ward, "Results of Test Coverage Analysis on the PARTISN QA Sets(U)," LANL internal memorandum, CCS-4:05-40, July, 2005.

R.C.Ward, "Software Requirements Specification for a Two-Dimensional Production Quality Block-Adaptive Mesh Refinement (AMR) with Diffusion Synthetic Acceleration (DSA) Solver in PARTISN(U)," LANL internal memorandum, CCS-4:05-59, November 2005.

S.W. Mosher, "Results of the SMORZ Project," LANL Memorandum CCS-4:05-18(U), LA-UR-05-2390, (March 30, 2005).

T.J. Urbatsch, "What it's like Pretending to Transport Radiation an overview of the Transport Methods Group at LANL," invited talk to the Nuclear Engineering Department at The Pennsylvania State University, LA-UR-05-1260, 2005.

T.J. Urbatsch, T.M. Evans, "Milagro Version 2, An Implicit Monte Carlo Code for Thermal Radiative Transfer: Capabilities, Development, and Usage," Los Alamos National Laboratory report LA-14195-MS, January 2005.

T.M. Evans, "An Interface for Domain Decomposition in Wedgehog (U)," CCS-4:05-74, December 7, 2005, Los Alamos National Laboratory, Research Note.

T.M. Evans, "Vision, Scope, and Implementation Plan for the Me Marval Project (U)," CCS-4:05-71, November 22, 2005, Los Alamos National Laboratory, Research Note.

T.M. Evans, J.D. Densmore, M.W. Buksas, A.L. Hungerford, S.W. Mosher, P.J. Henning, T.J. Urbatsch, "Release of ClubIMC-3_0_0," CCS-4:05-72, November 22, 2005.

T.M. Evans, J.D. Densmore, M.W. Buksas, A.L. Hungerford, S.W. Mosher, P.J. Henning, T.J. Urbatsch, "Release of Wedgehog-5_0_0," CCS-4:05-73, November 29, 2005, Los Alamos National Laboratory, Research Note.

T.M. Evans, J.D. Densmore, T.J. Urbatsch. "Equilibrium-Diffusion Material Motion Correction for Wedgehog(U)," CCS-4:05-06. January 19, 2005, Los Alamos National Laboratory, Technical Memorandum.

T.M. Evans, T.J. Urbatsch, M.W. Buksas, J.D. Densmore, "Spherical Surface Tally Interface for Wedgehog(U)," CCS-4:04-02 Revision 3, April 21, 2005.

T.M. Kelley, "Characterization of Implicit Monte Carlo projects, phase 1: serial performance of Milagro (U)," CCS-4:06-03, Feb. 7, 2006, Los Alamos National Laboratory, Technical Memorandum.

T.M. Kelley, "Planning Chimp-1: Milagro Serial (U)," CCS-4:05-61, Oct. 18, 2005, Los Alamos National Laboratory, Technical Memorandum.

T.M. Kelley, "Vision and Scope for Chimp-1: Milagro serial (U)," CCS-4:05-60, Oct. 18, 2005, Los Alamos National Laboratory, Technical Memorandum.


## CCS-4 Citation Indices (showing top 25 CCS-4 articles written for LANL in the last 10 years with number of times cited listed first)

(43) Y.C. Zhong, M.P. Sarachik, J.R. Friedman, R.A. Robinson, T.M. Kelley, H. Nakotte, A.C. Christianson, F. Trouw, S.M.J. Aubin, D.N. Hendrickson, "Inelastic neutron scattering study of Mn-12-acetate", J. Appl. Phys., 85, p. 5636-8 (1999).

(18) J.S. Warsa, M. Benzi, T.A. Wareing, J.E. Morel, "Preconditioning a mixed discontinuous finite element method for radiation diffusion," Numerical Linear Algebra With Applications; Oct-Nov 2004; v.11, no.8-9, p.795-811.

(17) D.N. Argyriou, T.M. Kelley, J.F. Mitchell, R.A. Robinson, R. Osborn, S. Rosenkranz, R.I. Sheldon, J.D. Jorgensen, "Two-dimensional ferromagnetic correlations above $T\_C$ in the naturally layered CMR manganite La_2-2x Sr_1+2x Mn_2 O_7 (x=0.3-0.4).", J. Appl. Phys., 83, p. 6374-8 (1998).

(13) S.A. Turner, E.W. Larsen, "Automatic Variance Reduction for Three-Dimensional Monte Carlo Simulations by the Local Importance Function Transform - II : Numerical Results", Nucl. Sci. Eng., 127, p.36-53, 1997.

(12) A. Hungerford, C. Fryer, M. Warren, "Gamma Ray Lines from Asymmetric Supernovae," The Astrophysical Journal, 594, 390, 2003.

(10) J.S. Warsa, T.A. Wareing, J.E. Morel, "Fully consistent diffusion synthetic acceleration of linear discontinuous SN transport discretizations on unstructured tetrahedral meshes," Nuclear Science and Engineering; July 2002; vol.141, no.3, p.236-51.

(10) S.A. Turner, E.W. Larsen, "Automatic Variance Reduction for Three-Dimensional Monte Carlo Simulations by the Local Importance Function Transform - I : Analysis", Nucl. Sci. Eng., 127, p.22-35 1997.

(8) R.S. Baker, K.R. Koch, "An Sn Algorithm for the Massively Parallel CM-200 Computer", Nucl. Sci. Eng, 128, p. 312-320, 1998.

(8) R.J. McQueeney, A.C. Lawson, A. Migliori, T.M. Kelley, B. Fultz, M. Ramos, B. Martinez, J.C. Lashley, S.C. Vogel, "Unusual phonon softening in {delta}-phase plutonium", Phys. Rev. Lett., 92, p. 146401/1-4 (2004).

(6) T.M. Kelley, W.P. Beyermann, R.A. Robinson, F. Trouw, P.C. Canfield, H. Nakotte, "Crystal-field spectrum and linewidths in the heavy-fermion system PrInAg_2 ", Phys. Rev. B, 261, p.1831-5 (2000).

(5) K.A. Van Riper, T.J. Urbatsch, P.D. Soran, D.K. Parsons, J.E. Morel, G.W. McKinney, S.R. Lee, L.A. Crotzer, F.W. Brinkley, T.E. Booth, J.W. Anderson, R.E. Alcouffe, "AVATAR - Automatic variance reduction in Monte Carlo calculations," Proceedings 1997 Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications, Saratoga Springs, New York, October 6-10, 1997, vol. 1, p. 661.

(4) J.S. Warsa, T.A. Wareing, J.E. Morel, "Solution of the discontinuous P-1 equations in two-dimensional cartesian geometry with two-level preconditioning," SIAM Journal On Scientific Computing; 2003; v.24, no.6, p.2093-2124.

(4) T.M. Kelley, D.N. Argyriou, R.A. Robinson, H. Nakotte, J.F. Mitchell, R. Osborn, J.D. Jorgensen, "Short Range Spin Correlations in the CMR Material La_1.4Sr_1.6Mn2O7", Physics B, 241-3, p.439-41 (1997).

(3) M.G. Gray, R.M. Roberts, T.M. Evans, "Shadow-object interface between F95 and C++," Computing in Science and Engineering, 1(2), 1999.

(3) P. Javorsky, H. Nakotte, R.A. Robinson, T.M. Kelley, "Crystal field in ErNiAl studied by inelastic neutron scattering", Journal of Magnetism and Magnetic Materials, 186, 373-6 (1998).

(2) J.S. Warsa, T.A. Wareing, J.E. Morel, J.M. McGhee, R.B. Lehoucq, "Krylov subspace iterations for deterministic k-eigenvalue calculations," Nuclear Science and Engineering; May 2004; vol.147, no.1, p.26-42.

(2) J.S. Warsa, A.K. Prinja, "p-adaptive numerical methods for particle transport," Transport Theory and Statistical Physics; 1999; vol.28, no.3, p.229-70.

(2) K.G. Thompson, M.L. Adams, "A Spatial Discretization for Solving the Transport Equation on Unstructured Grids of Polyhedra," Proceedings for the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, 27 30 September 1999; Madrid, Spain.

(2) T.J. Urbatsch, R.A. Forster, R.E. Prael, R.J. Beckman, "Estimation and Interpretation of Keff Confidence Intervals in MCNP," Nuclear Technology, 111:169-182, 1995.

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(1) J.A. Dahl, "A Non-Linear Method for Representing the Scattering Cross Section for Discrete Ordinates", Proceedings of The Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications, Saratoga Springs, NY, Vol 2, p.1497-1506, October 5-9, 1997.

(1) J.S. Warsa, "Analytical SN solutions in heterogeneous slabs using symbolic algebra computer programs," Annals of Nuclear Energy; May 2002; vol.29, no.7, p.851-74.

(1) J.S. Warsa, T.A. Wareing, J.E. Morel, "Krylov iterative methods and the degraded effectiveness of diffusion synthetic acceleration for multidimensional S-N calculations in problems with material discontinuities," Nuclear Science and Engineering; Jul 2004; vol.147, no.3, p.218-248.

(1) M.W. Buksas, "Implementing the Perfectly Matched Layer Absorbing Boundary Conditions with Mimetic Differencing Schemes," Progress in Electromagnetics Research 2001; v.32 p. 383-411.

(1) T.M. Evans, T.J. Urbatsch, H. Lichtenstein, J.E. Morel, "A residual Monte Carlo method for discrete thermal radiative diffusion," Journal of Computational Physics, Volume 189, Issue 2, August 2003, Pgs 539 - 556.

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(1) T.M. Evans, T.J. Urbatsch, and H. Lichtenstein, "1-D Equilibrium Discrete Diffusion Monte Carlo," Proceedings of the International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation, and Applications. Lisbon, Portugal, October 2000.

## CCS-4 Participation on Review and Advisory Committees

J.A. Dahl, L2 Review Committee, "High Fidelity Multigroup Nuclear Data Library," 2005.

R.S. Baker, L2 Review Committee, "A Specific Transport Capability In-line in Projects A and B," 2005.

R.S. Baker, L2 Review Committee, "Primary V&V," 2005.

T.J. Urbatsch, L2 Review Committee, "Software Quality Project," 2005. With Laura McClellan, X-8, chair; Larry Cox, ADWP; and David Pimentel, CCN-12. The milestone material and presentation were given by Rob Kelsey, CCN-12. The review was held August 25, 2005.