

Nuclear Engineering Research Projects 2006-07

NSINEMA: Simulation Institute for Nuclear Energy Modeling and Analyses

Paul Turinsky and Hany Abdel-Khalik
Idaho National Laboratory
\$230,000
4/1/05 – 9/30/07

The overall goal of SINEMA is to provide a computational tool for decision makers in regard to evaluating alternative nuclear fuel cycles, with assessments of their cost, proliferation resistance, final waste disposal impact, nuclear safety and time-line implementation feasibility. To accomplish this objective, the total nuclear fuel cycle from birth (mining) to death (final disposal) must be computationally modeled. NC State's portion of this joint INL, ANL and NC State project is to develop the capability to assess the uncertainties in key performance metrics due to input data and eventually modeling uncertainties.

Managing Model Data Introduced Uncertainties in Simulator Predictions for Generation IV Systems via Optimum Experimental Design

Paul J. Turinsky and Hany Abdel-Khalik
Department of Energy
\$399,218
4/1/06 – 3/31/09

The proposed research addresses the understanding and management of uncertainties that originate due to the uncertainties of physical data that are utilized in modeling and simulation software, i.e. model data. The research will address the quantification of uncertainties and the optimum design of experiments that reduce these uncertainties. An advanced Generation IV reactor core's uncertainties will be assessed and a simulation of the INL ZPPR critical facility will be utilized as the pseudo-experimental facility to reduce these uncertainties, to test the mathematical capabilities developed.

Analysis of Curvilinear Geometry Characteristic-Based Particle Transport Discretizations

Dmitriy Anistratov
Lawrence Livermore National Laboratory, US DOE
\$35,000,
09/01/06-08/30/07

The goal of this project is to investigate the properties of a variety of characteristic methods in 1D spherical and cylindrical geometry. We will analyze the behavior of the discretizations in optically-thick and diffusive regions, using the asymptotic diffusion limit analysis, the infinite-medium low-order polynomial solutions, as well as a variety of special test problems. The expected results of this research will form the background for development of accurate and robust transport methods for r-z geometry and will be used to determine the next step in this direction.

Nonlinear Projective-Iteration Methods for Solving Transport Problems on Regular and Unstructured Grids

Dmitriy Anistratov
Nuclear Engineering Education Research, US Department of Energy
\$357,235
6/1/03 – 1/31/07

The goal of the project is to make significant progress in creating efficient methods for solving multidimensional transport problems. The transport equation is a background for mathematical models of particle transport in nuclear reactors, radiative transfer in plasmas, well-logging problems etc. Except for highly idealized models, it can be solved only by means of numerical methods. The project will focus on development of unconditionally stable methods for solving the multidimensional transport equation on unstructured grids and new nonlinear methods with advanced properties and adaptive features for regular meshes based on nonlinear projective-iterative methods, namely, the Quasidiffusion and Yvon-Mertens methods.

Production and Application of Novel Insecticidal and Antimicrobial Textiles Using Atmospheric Plasmas and Irradiation Techniques

Mohamed Bourham (USA) and Samiha Gawish (Egypt)
NSF International / US State Department
\$65,613 (\$33,213 US PI M. Bourham and \$32,400 Egypt Co-PI)
9/01/03 – 8/31/06

Advanced atmospheric plasma-aided techniques applied to textile materials to develop biocidal textiles. Functionalization of textile materials with atmospheric plasma provides three distinctive features, antimicrobial, insect repellent and antistatic properties. Fabrics activation by plasma followed by a developed copolymerization grafting method adopted in this project for the formation of bioactive sites onto the textiles without impairing their original mechanical properties. These novel biocidal textiles include antimicrobial fabrics, mothproof wool and insect repellent fabrics.

Plasma-Aided Antimicrobial/Insect Repellent Finishing

Marian McCord and Mohamed Bourham
Institute of Textile Technology (ITT)
\$56,000
05/01/05 – 05/15/06

Atmospheric plasma-enhanced graft copolymerization of bioactive monomers onto the fabric, followed by addition of insecticidal antimicrobial agents is investigated. In preparation for chemical grafting, oxygenated helium plasma is used to expose fabric samples to helium and oxygen ions, creating active sites on the fabric surface. Fixation of insecticidal agents into the cavity of the antimicrobial agents adds a second protective feature to the product. Grafted fabrics are washed and tested for antimicrobial and insecticidal/insect repellent properties.

Stain Repellent-Antimicrobial Textiles via Atmospheric Plasma Finishes

Marian McCord and Mohamed Bourham
Institute of Textile Technology (ITT)
 \$63,965
 07/01/06 – 06/30/07

Stain repellent antimicrobial finishes are extremely important to provide protection against microbial attacks and to prevent the threat of cross-transmission of diseases from spilled human fluids. Atmospheric plasma activation of fabrics with in-situ graft copolymerization of bioactive monomers is an efficient, low-cost, durable and permanent method to provide antimicrobial textiles. An additional feature using plasma technique is to also provide a barrier finish against stains, either soil or drinking fluids. Stain repellency of body fluids is also important to eliminate cross transmission of diseases.

On-Line Fuel Failure Monitor for Fuel Testing and Monitoring of Gas Cooled Very High Temperature Reactors

Ayman I. Hawari and Mohamed A. Bourham
US Department of Energy
 \$498,429
 03/25/05 – 03/24/08

In the Very High Temperature Reactor, the fuel is based on the concept of the TRISO microsphere. The microsphere is composed of a UO₂ kernel surrounded by a porous pyrolytic graphite buffer, an inner pyrolytic graphite layer, a silicon carbide (SiC) coating, and an outer pyrolytic graphite layer. The enrichment of the fuel is expected to range from 4%– 10% in U-235. Due to the hostile in-core conditions, it is anticipated that a certain number of TRISO microspheres will fail during reactor operation. We will study the development of fuel failure detection methods using passive gamma-ray spectrometry.

Development of an Intense Positron Annihilation Spectroscopy System for Nanophase Characterization

Ayman Hawari, Mohamed Bourham, David Gidley, K. Linga Murty and Jun Xu
National Science Foundation
 \$999,563
 07/01/05 – 06/30/2008

Positron, with its affinity for open structures in matter, has been gaining an important role as a probe of nanostructure and in understanding the role of engineered nanovoids on macroscopic properties. Controlling and understanding the structure and behavior of vacancies and voids within a material requires understanding how the interaction between vacancies and impurities affects macroscopic properties. This major research is collaborative between NCSU, ORNL and University of Michigan to develop an intense positron beam facility at the NCSU PULSTAR reactor.

Thermohydraulic Modeling of Thermosyphon Cyclotron Targetry to Improve F-18 Clinical PET

J. Michael Doster
NIH (Phase II SBIR)
 \$198,892
 8/15/05 – 8/14/07

Bruce Technologies is involved in efforts to develop high performance cyclotron targetry for the production of F-18 for clinical Positron Emission Tomography (PET). Its production is limited by the ability to remove heat from the target. High performance targets with greater heat removal capabilities would allow for higher proton beam currents with associated higher production rates of the F-18 ion. A target design using boiling batch thermosyphon is being developed using thermohydraulic predictive models, which are correlated with experimental data of target performance and used to improve and optimize the target design for applications to a variety of accelerators.

Thermohydraulic Modeling of Recirculating Cyclotron Targetry to Improve F-18 Clinical PET

J. Michael Doster
NIH (Phase II SBIR)
 \$198,892
 8/15/05 – 8/14/07

Bruce Technologies is involved in efforts to develop high performance cyclotron targetry for the production of F-18 for clinical Positron Emission Tomography (PET). Its production is limited by the ability to remove heat from the target. High performance targets with greater heat removal capabilities would allow for higher proton beam currents with associated higher production rates of the F-18 ion. A target design using recirculating water targets is being developed using thermohydraulic predictive models, which are correlated with experimental data of target performance and used to improve and optimize the target design for applications to a variety of accelerators.

New Cyclotron Targetry to Enhance F-18 PET

J. Michael Doster
USDOE (NEER)
 \$347,184
 6/01/04 – 5/31/07

This project proposes to develop cyclotron targets that produce F-18 for clinical Positron Emission Tomography (PET) at significantly higher rates than available from current targetry. The beam power available in many commercial cyclotrons exceeds the capacity of current target technology by a factor of two to four. New target systems would allow a substantial increase in effectiveness of the approximately 250 PET cyclotrons now operating in the US. Cyclotron manufacturers will probably sell 25-50 new cyclotrons per year in the next few years. If new targets are available and utilized, they will offer a dramatic increase in production of F-18.

Associates Program for Nuclear Techniques in Oil Well Logging

Robin Gardner
Members: Baker Atlas, EXXON Mobil, Halliburton, Weatherford International, and Los Alamos National Laboratory
 \$100,000
 01/01/06 – 12/31/06

This program supports research and development in the oil well logging industry. Present work includes Monte Carlo simulation of horizontal and near horizontal logging while drilling (LWD) gamma-ray density and neutron porosity logs to establish environmental correction factors for them and the investigation of the Monte Carlo – Library Least-

Squares (MCLS) approach and unique coincidence well detectors for improving carbon/oxygen (C/O) log sensitivity. Received a computer cluster from Weatherford worth \$100,000

Developing an Inverse Approach to Monitoring for Special Nuclear Materials

Robin Gardner
Raytheon Tech
\$100,000
07/01/07– 06/30/08

Develop mathematical methods and tools, using the LANL MCNP/MCNPX or similar types of Monte Carlo codes, and procedures to accurately model gamma ray scintillation detector response functions (DRF) based on the specific detector geometry, scintillator material and PMT and surrounding materials of construction. Integrate these developed patches into the Raytheon MCNP/MCNPX code package. Developing an iterative technique that estimates how much of each identified radioisotope is in the spectrum. This method would also include a non-linear estimate of the amount and type of shielding that is involved.

Multi-University Southeast INIE Consortium

Ayman I. Hawari
US Department of Energy
\$5,867,298
09/10/03 – 09/09/08

The Multi-University Southeast INIE Consortium (MUSIC) was established in response to the US Department of Energy's (DOE) Innovations in Nuclear Infrastructure and Education (INIE) program. MUSIC is a consortium composed of academic members and national laboratory partners. The members of MUSIC are the nuclear engineering programs and research reactors of: University of Florida (UF), Georgia Institute of Technology (GIT), North Carolina State University (NCSU), University of Maryland (UMD), University of Tennessee (UTK), and University of South Carolina (USC). In addition there are three university research reactors (URRs) within MUSIC, which are located at NCSU (1-MW PULSTAR), UMD (0.25-MW TRIGA) and UF (0.1-MW Argonaut).

Molecular Dynamic Analysis of Radiation Damage in Graphite and Silicon Carbide

Ayman I. Hawari
Idaho National Laboratory
\$109,000
12/21/04 – 12/31/06

Graphite and Silicon Carbide are key materials for the development of the Very High Temperature Reactors. In this work, classical molecular dynamics methods are developed and implemented for simulating radiation damage in these materials. Using these simulations, the temperature dependent threshold displacement energy is calculated for subsequent use in the calculation of damage rates. For graphite, the resultant structures are used in atomistic simulations to study the impact of damage on thermal neutron scattering in these materials.

Development of an Intense Positron Annihilation Spectrometry System for Nanophase Characterization

Ayman I. Hawari, Mohamed A. Bourham, K. L. Murty, David Gidley (UM), Jun Xu (ORNL)
National Science Foundation
\$999,563
09/01/05 – 08/31/08

The intense positron beam at NCSU will drive two complementary positron/positronium spectrometers: First, a "next generation" positronium PALS spectrometer (Ps-PALS), with a 1-mm diameter beam, that is capable of performing high accuracy lifetime studies on nanoporous thin films and patterned microelectronic devices., and second, a time-bunched positron PALS spectrometer (e+-PALS) that will be directed for studying annihilation in metals and semiconductor. A prototype positron beam has been designed, built and is currently being tested at the PULSTAR reactor. The positron beam facility will have applicability in fields such as materials science and engineering, biomedical engineering, chemical engineering, electrical engineering, environmental science and engineering, physics and chemistry.

On-Line Fuel Failure Monitor for Fuel Testing and Monitoring of Gas Cooled Very High Temperature Reactors US Department of Energy

Ayman I. Hawari and Mohamed A. Bourham
\$498,429
03/25/05 – 03/24/08

In the Very High Temperature Reactor, the fuel is based on the concept of the TRISO microspheres. The microsphere is composed of a UO₂ kernel surrounded by a porous pyrolytic graphite buffer, an inner pyrolytic graphite layer, a silicon carbide (SiC) coating, and an outer pyrolytic graphite layer. The enrichment of the fuel is expected to range from 4% – 10% in U-235. Due to the hostile in-core conditions, it is anticipated that a certain number of TRISO microspheres will fail during reactor operation. We will study the development of fuel failure detection methods using passive gamma-ray spectrometry.

A High Accuracy Approach for the Efficiency Characterization of HPGe Detectors in an Extended Energy Range

Ayman I. Hawari
Los Alamos National Laboratory
\$183,783
10/01/02 – 07/31/07

This project develops a hybrid experimental/computational approach for the high accuracy characterization of the relative efficiency curve of HPGe detectors. Monte Carlo simulations will be used to design a prompt gamma-ray detector calibration source, and to establish a relative efficiency curve. The experimental part will determine a high accuracy relative efficiency curve for the HPGe detector, which in combination with the Monte Carlo results can extend from 100 keV to 10,000 keV. We will study the use of curve fitting methods that would enable the determination of accurate analytical expression for the relative efficiency curve over an extended energy range.

Design Simulations and Testing of a Gaseous Electron Multiplier Neutron Detector

Ayman I. Hawari

Instrumentation Associates / US Department of Energy
\$106,142

03/21/05 – 06/30/07

Design simulations and preliminary testing will be performed to study the characteristics of a gaseous electron multiplier (GEM) detector. This device employs a Gd/CsI neutron converter screen and GEM electron amplifiers as the central elements of a high resolution time and position sensitive thermal neutron detector. The device, once operational, is planned to be implemented at the Spallation Neutron Source (SNS) facility of Oak Ridge National Laboratory. The testing of the detector will be performed at the PULSTAR reactor of North Carolina State University.

Implications of Graphite Radiation Damage on the Neutronic, Operational, and Safety Aspects of Very High Temperature Reactors,

Ayman I. Hawari

US Department of Energy
\$568,879

06/01/07 – 05/31/10

In the prismatic and pebble bed designs of Very High Temperature Reactors, the graphite moderator is expected to reach exposures of 1021 to 1022 n/cm² over the reactor lifetime. This exposure results in damage to the graphite structure. Studies of the thermal properties of irradiated graphite show changes in the thermal conductivity and (to a lesser extent) the heat capacity at fluences less than 1021 n/cm². These properties depend on the behavior of atomic vibrations (phonons) in the solid. Therefore, it can be expected that any alterations in the phonon behavior that would produce changes in these properties would have an impact on thermal neutron scattering.

Deformation Microstructures and Creep Mechanisms in Advanced Zr-based Cladding under Biaxial Loading

K.L. Murty

Department of Energy
\$299,874

7/1/04 – 6/30/07

The proposal addresses characterization of anisotropic biaxial creep and transitions in creep mechanisms of advanced cladding alloys considered for high burn-up applications in light water reactors. The new generation alloys include additions of niobium, vanadium along with slight changes in alloy chemistry as well as barrier cladding with and without low tin on the surface. The study is mainly to characterize crystallographic textures and investigate creep behavior under biaxial loading along with the development of CODF-creep models to predict their complex deformation behaviors. Particular attention is paid to transitions in creep mechanisms as lower stresses are encountered.

Effect of Alloying and Thermo-mechanical Treatment on Anisotropic Creep and Deformation of Ti-Alloys

K.L. Murty and R.O.Scattergood

National Science Foundation
\$500,000

9/1/04 – 8/31/08

The proposal addresses the influence of thermo-mechanical-treatment (TMT) and alloying on deformation and creep anisotropy of titanium alloys. The study involves characterization of anisotropic biaxial creep of Ti alloys using closed-end internally pressurized thin-walled tubing superimposed with axial load. Cold-working leads to grain-shape anisotropy of the otherwise equiaxed grain structure of Rx materials. The effects of these variables on the deformation microstructures will be investigated along with deformation anisotropy following biaxial loading under varied stress-states and stress-levels. This is a renewal proposal of the project funded in 2001.

A Multiscale Study of Ratcheting Failure Mechanisms in Austenitic and Ferritic Steel Welded Joints

Tasnim Hassan and K.L. Murty

National Science Foundation
\$319,000

9/1/04 – 8/31/07

The main objective of the proposed study is to investigate the causes for the ratcheting fatigue failures of welded joints. It is anticipated that it is caused by either the residual stresses and/or heterogeneity in the dislocation substructures of welded joints. Under this grant support, a systematic set of fatigue tests on welded joints will be conducted and residual stresses will be measured at various stages of fatigue lives. A major part involves an investigation on the micro-structural processes of welded joint fatigue failures. The relationship between multiscale fatigue mechanisms of welded joints will be explored.

INT-collaboration: Creep Anisotropy in Titanium – Textural and Microstructural Origin

K.L. Murty

National Science Foundation
\$40,170

9/1/04 – 8/31/07

The grant will enable a collaborative research between North Carolina State University, USA and Indian Institute of Technology, Mumbai, India, for an investigation on the anisotropic deformation behavior of titanium and its alloys. Microtextural studies at IIT along with microstructural aspects will be related to the macroscopic behaviors. Quantitative models will be developed based on both preferred orientations and the microstructural details to predict the dimensional changes of structures made of these materials. The international collaboration is expected to lead to an understanding and development of textured Ti alloys that find application in aerospace, biomedical and other technologies.

Nuclear Fuel Management Optimization: FORMOSA-P and -B Codes

Paul Keller and Paul Turinsky

Electric Power Research Center, NC State University
\$98,749 (total \$3,300,000 since project initiation)

01/01/05 – 12/31/06

The FORMOSA-B and -P code were developed to complete incore nuclear fuel management optimization for boiling water reactors (BWRs) and pressurized reactors (PWRs), respectively. The incore problem's decision variables concern placement and loading within the core of fuel, burnable poisons, and for BWRs control rods as a function

of exposure. Operational and safety limits are imposed as constraints. The FORMOSA series of codes combine a core simulator and optimization methodology. Single and Multiple Objective Simulated Annealing or Genetic Algorithm can be employed as the optimization method. The core simulator solves the two-group, two- or three-dimensional neutron diffusion equation utilizing either the nodal expansion method or semianalytic method.

SINEMA: Simulation Institute for Nuclear Energy Modeling and Analyses

Paul Turinsky and Hany Abdel-Khalik
Idaho National Laboratory
\$230,000
4/1/05 – 9/30/07

The overall goal of SINEMA is to provide a computational tool for decision makers in regard to evaluating alternative nuclear fuel cycles, with assessments of their cost, proliferation resistance, final waste disposal impact, nuclear safety and time-line implementation feasibility. To accomplish this objective, the total nuclear fuel cycle from birth (mining) to death (final disposal) must be computationally modeled. NC State's portion of this joint INL, ANL and NC State project is to develop the capability to assess the uncertainties in key performance metrics due to input data and eventually modeling uncertainties.

Establishment, Planning and Development Activities for Academic Center of Excellence in Advanced Modeling and Simulation

Paul Turinsky
Idaho National Laboratory
\$325,000
2/1/05 – 9/30/07

This project is to establish the Academic Center of Excellence in Advanced Modeling and Simulation (ACE-AMS). At INL, the Center for Advanced Modeling and Simulation (CAMS) is being established. ACE-AMS will complement CAMS, focusing on conducting research on developing computational capabilities to understand how modeling and data uncertainties propagate through sophisticated models of physical processes and impact the uncertainties of key integrated system performance attributes.

Development and Utilization of Mathematical Optimization in Advanced Fuel Cycle Systems Analysis

Paul Turinsky
Department of Energy
\$321,698
4/1/06-3/31/09

This project proposes to develop the capability to determine the optimum deployment strategies for advanced reactor/fuel/fuel cycle facilities for the nation within constraints utilizing mathematical optimization. A stochastic optimization approach will be employed, which will allow the tradeoff surface of this multi-objective optimization problem to be determined. Economic, energy, environmental and nonproliferation resistance metrics of the fuel cycle will be considered in the optimization. The VISION code will be employed to model the fuel cycle.

Managing Model Data Introduced Uncertainties in Simulator Predictions for Generation IV Systems via Optimum Experimental Design

Paul J. Turinsky and Hany Abdel-Khalik
Department of Energy
\$399,218
4/1/06 – 3/31/09

The proposed research addresses the understanding and management of uncertainties that originate due to the uncertainties of physical data that are utilized in modeling and simulation software, i.e. model data. The research will address the quantification of uncertainties and the optimum design of experiments that reduce these uncertainties. An advanced Generation IV reactor core's uncertainties will be assessed and a simulation of the INL ZPPR critical facility will be utilized as the pseudo-experimental facility to reduce these uncertainties, to test the mathematical capabilities developed.

Scoping Study Addressing Potential Manners of Reducing Nuclear Fuel Cycle Costs for the Palo Verde Nuclear Generating Station

Paul J. Turinsky
Arizona Public Service Corporation
\$101,270
9/1/06 – 8/31/07

Nuclear fuel cycle costs, which makeup approximately one-third of generating costs for nuclear power plants, have been increasing as of recent because of mainly the increasing price of uranium ore. Over the past three years, uranium ore prices on the spot market have increased substantially. This scoping study will assess what improvements can be made in fuel cycle costs via changes in the fuel assembly design and fuel management practices, considering replacement power costs where applicable, and the difficulty of making such improvements considering the issues of implementation cost, engineering effort, maturity of technology, and licensing and plant modifications required. This scoping study will be completed for the Palo Verde Nuclear Generating Station.

Feasibility of Electron Accelerators for Nuclear Waste Transmutation

Man-Sung Yim
Russell Family Foundation
\$158,175
10/01/01 – 9/30/07

This research examines feasibility of the electron accelerator-based nuclear waste transmutation. For this purpose, comparative assessment of nuclear waste transmutation technology was performed between the proton accelerator-based system and the electron accelerator-based system. A conceptual design of an electron accelerator driven transmutation (sub-critical core) system is developed for this purpose. Performance of the systems is compared with respect to neutron yield characteristics, transmutation efficiency, and net power generation. Other performance characteristics such as cost, safety/reliability of the system are examined.

Investigation of Optimum Method for Nuclear Waste Transmutation

Man-Sung Yim
Russell Family Foundation
 \$121,840
 10/01/03 – 9/30/07

The objective of this research is to develop a methodology for the selection of optimum nuclear waste transmutation system. Quantitative models have been developed to assess key performance measures of the system, i.e., transmutation efficiency, economics, repository impacts, and proliferation resistance. Examples of proposed technologies for the transmutation of nuclear waste were evaluated and compared.

Characterization of Radiological Risk from Former Nuclear Weapons Sites in Russia

Man-Sung Yim
Russell Family Foundation
 \$34,390
 10/01/06 – 9/30/07

The objective of this research is to perform radiological risk assessment on the Russian Research Center Kurchatov Institute located in Moscow and to develop guidelines for risk management decision making.

Development of a Bayesian Method for the Detection of Nuclear Proliferation

Man-Sung Yim
Idaho National Laboratory
 \$178,000
 06/01/06 – 9/30/08

The objective of this research is to design, develop, and demonstrate a Bayesian-based decision support system for identification of situations where the operator of a nuclear fuel cycle facility may plausibly be either preparing for or participating in nuclear proliferation. Extensive investigations on why and why not certain countries have attempted diversion are performed. Presently the information for various events of interest are being utilized to derive the necessary prior probability distributions to characterize proliferation decision.

NUCLEAR ENGINEERING FACULTY

Mohamed A. Bourham, Professor of Nuclear Engineering and Interim Department Head, (919.515.7662); PhD Ain Shams University, Egypt 1976; Plasma-Matter Interaction, plasma-driven Launchers, fusion engineering, industrial plasmas, low temperature and non-ideal plasmas, charged particle beams and electron irradiation systems, atmospheric and industrial plasmas, x-ray sources for medical and screening imaging. [bourham@ncsu.edu]

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Paul J. Turinsky, Professor of Nuclear Engineering and Director of the Electric Power Research Center (919.515.5098); PhD University of Michigan 1970; Nuclear fuel management optimization, advanced nuclear fuel cycles, computational efficient solution of coupled neutronic/thermal-hydraulic reactor core problems, and space-time neutron kinetics. [turinsky@ncsu.edu]

Man-Sung Yim, Director of Graduate Programs and Associate Professor of Nuclear Engineering (919.515.1466); PhD University of Cincinnati 1987; Sc.D. Harvard University 1994; Nuclear waste management, risk assessment, radiological health. [yim@ncsu.edu]

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