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High-Fidelity Space-Time Adaptive Multiphysics Simulations in Nuclear Engineering

Fuel Cycle R&D

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Nuclear Energy University Programs
U.S. Department of Energy

High-Fidelity Space-Time Adaptive Multiphysics Simulations in Nuclear Engineering

Final Report, DOE/NEUP Award 09391

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Summary of deliverables

For reference we present the following summary of deliverables:

"We will deliver a new methodology for space-time adaptive high-order monolithic discretization of arbitrary time-dependent multiphysics PDE problems in nuclear engineering. We will also deliver a new software architecture that allows for simple plug-and-play assembly of arbitrary multiphysics PDE systems, and their solution via space-time adaptive higher-order methods on dynamical meshes. Demonstrative examples will include (i) reactor transients, (ii) coupled heat conduction and oxygen diffusion in fuel rods, and (iii) coupled neutron diffusion/heat conduction/single phase fluid flow."

More information including detailed annual plans can be found in Appendix A - F.

Summary of most important results delivered

We delivered a series of fundamentally new computational technologies that have the potential to significantly advance the state-of-the-art of computer simulations of transient multiphysics nuclear reactor processes. These methods were implemented in the form of a C++ library, and applied to a number of multiphysics coupled problems relevant to nuclear reactor simulations.

Monolithic adaptive multimesh hp-FEM discretization of multiphysics coupled problems

This method makes it possible to perform higher-order finite element approximations of nonlinear time-dependent multiphysics coupled problems using individual meshes for every physical field. In contrast to usual operator-splitting (OS) techniques that suffer from accuracy and stability problems, the multimesh hp-FEM method provides a monolithic approximation without breaking any physics in the model. In other words, the multimesh hp-FEM treats the multiphysics PDE system as one vector-valued equation. The only error made during the discretization is an error in numerical quadrature, which is inherent to all finite element discretizations. There is no decoupling of equations in the system or anything of this sort. The meshes for all physical fields evolve in time adaptively and independently of each other. References: [1, 2, 12, 15].

Monolithic coupling of hp-FEM and hp-DG methods

The multimesh hp-FEM was generalized to allow some physical fields in a multiphysics coupled problem to be approximated using hp-FEM and others using hp-DG. The resulting discretization is again monolithic, meaning that no physics is lost. Such a combination of hp-FEM and hp-DG is particularly desirable in nuclear reactor problems that include flows, which are better approximated using Discontinuous Galerkin (DG) methods rather than Finite Element methods (FEM). References: [4].

New modular approach to higher-order time discretization of transient PDE problems

Traditionally, a transient PDE solver implements one, or at most a few, different time integration methods. Our new method makes it possible to enter the time integration method as an additional parameter of the PDE solver. In other words, the spatial and temporal discretizations are completely decoupled. The huge benefit of this approach is that any PDE or multiphysics coupled PDE system can be solved using many different time integration methods – explicit or implicit, low-order or high-order - without altering the computer code of the PDE solver. In particular, our method makes it easy to apply embedded adaptive higher-order implicit Runge-Kutta methods to arbitrary multiphysics coupled problems. References: [13, 15].

New class of iterative methods for the adaptive solution of eigenproblems

We developed a novel approach to automatic adaptivity in the finite element discretization of eigenproblems. When solving eigenproblems adaptively, the usual approach has been to use the same mesh for all eigenfunctions. Since eigenfunctions often have large qualitative and quantitative differences, this approach is inefficient. Our new method makes it possible to approximate every eigenfunction on an individual mesh, and also, to pursue only one or a few selected eigenfunctions, incontrast to the standard approach where always N eigenfunctions must be computed. References: [14, 16].

Plug-and-play software architecture for the solution of multiphysics problems

We also designed a corresponding plug-and-play software architecture for the solution of multiphysics problems, and implemented it in the form of a C++ library Hermes. The library is available at `http://hpfem.org/hermes`. References: [16]. The Co-PI applied some of the above-mentioned methods to reactor simulations: [3, 6, 7, 8, 9, 10, 11]

Solution progress and obtained results

2010 - Quarter 3

We have added automatic adaptivity to the multigroup one-dimensional examples that we created in the second quarter. We continued adjusting the PIs software system Hermes2D to be better usable as a common software platform for the PI and Co-PI. Interface to nonlinear solvers was improved. Space-time adaptivity with dynamical meshes was added to the 2-group neutronics example that was implemented in the second quarter with Co-PIs student Damien Lebrun. Currently we are in the middle of major changes of the Hermes2D library. So far Hermes2D has been able to assemble linear and nonlinear systems of equations (one stiffness or Jacobian matrix, one right-hand side or residual vector). Currently it is not possible to solve generalized eigenproblems which require the assembling of two matrices. Therefore we have separated the assembling and solver parts of the code, and exposed to the user data structures for the matrices and vectors. The work on these changes will continue in the fourth quarter and after they are finished, the user will be able to assemble as many matrices and vectors as he needs. Assembling will be done into structures provided by the user, such as PETSc, Trilinos, and other data structures. After assembling, the user will be able to call a variety of linear and nonlinear solver. We wrote several internal tests for the neutronics functionality in Hermes2D in harmony to the proposal objectives.

2010 - Quarter 4

In the second quarter we restructured the Hermes1D code to handle multigroup and multimaterial problems. A new example for a 2-group, 7-material eigenproblem was created. Most of work in the second quarter was done on the two-dimensional solver Hermes2D. A Co-PI's student Damien Lebrun-Grandie from Texas A&M visited my group on April 9 - 13 and we worked together on a new time-dependent benchmark example for coupled neutronics and heat transfer. An implicit Euler time stepping was implemented for this example. The example is not adaptive yet but its big advantage is that it comes with a known (manufactured) exact solution. Therefore it will become the basis for testing and debugging space-time adaptive algorithms. By doing this, we made a significant progress to the main objective for the first year, which is to "solve the nonlinear neutronics-thermal coupled problem efficiently and with controlled accuracy in both space and time via space-time adaptive multimesh hp-FEM." With my assistance, the Co-PI learned a lot about the Hermes2D code and started to adjust his own code Karma to interface Hermes2D. The Co-PI started to use the mailing list of my group and the git repository of Hermes2D. This means that both teams now share a common software development platform which is very good for future progress. Since there are many technical things to be done before the softwares are fully compatible, it is expected that this process will continue for the rest of the year. This corresponds to the proposal timetable: "Establishing a common software platform is an important milestone to be reached during the first year of the project."

2011 - Quarter 1

Rebuilding of the internal structure of the Hermes library We finished rebuilding of the internal structure as well as the Application Programming Interface (API) of the software package Hermes. These changes were necessary to enable plug-and-play architecture where various modules and external packages can be switched easily. Merging code repositories of Hermes1D, Hermes2D and Hermes3D The code repositories of Hermes1D, Herms2D and Hermes3D were merged into a single repository Hermes, and common functionality such as matrix solvers, error handling, logging, and time measurement were extracted into a new module called hermes_common. This further simplified the structure of the library and improved its usability. Variety of matrix solvers enabled Before we only used a direct sparse matrix solver UMFPACK to solve matrix problems arising in the hp-FEM discretization. During this quarter we added interfaces to the matrix solver packages Amesos, AztecOO, MUMPS, PARDISO, PETSc, SuperLU, and a matrix-free JFNK solver NOX from the Trilinos package. New Trilinos examples created We created five new examples illustrating how to use the Trilinos library. For each example we created an internal test. Solution of eigenproblems enabled We created several new examples for the solution of generalized eigenproblems. Enabling this functionality was one of the main reason why we started rebuilding the library in the last quarter. Adaptive multimesh hp-FEM extended to four group neutronics Adaptive multimesh hp-FEM for a two-group benchmark with analytic solution was extended to a four-group neutronics problem. Several higher-order time integration methods added We implemented and tested four different time integration methods that are second-order accurate in time: the Crank-Nicolson method, two second-order implicit BDF methods, and a Singly Diagonally Implicit Runge-Kutta method (SDIRK-22). Time integration with adaptive choice of time step was implemented in two versions: using the so-called PID controller, and using the pair of second-order BDF formulas whose combination yields a method that is third-order accurate in time. Newton method compared with Picard (fixed point) iteration The CoPI compared the merits of Newton method versus Picard iteration (fixed point iteration) to solve nonlinear problems arising from the discretization of PDEs. Many new internal tests added for quality assurance To assure quality of the software library, many new internal tests for the newly added functionality were implemented. The Hermes library has now around 500 internal tests that ensure its correctness and stability, and facilitate team development. Algorithmic basis for higher-order Discontinuous Galerkin)hp-DG) methods implemented We started the develop Training three graduate students in FEM and nuclear reactor modeling Continued training three graduate students on finite element technology, software development, and nuclear reactor modeling. Creation of a new graduate-level course at UNR related to nuclear engineering In the Fall semester 2010 the PI is teaching for the first time a new course "Advanced Computer Modeling in Engineering Applications" at UNR that he proposed and created in collaboration with INL staff. In this course, students are exposed to mathematical foundations of finite element analysis, mesh generation, and scientific visualization related to nuclear reactor modeling. They have to implement a simpler 2D finite element code by themselves, and their semester projects includes solving a realistic 3D problem using the Hermes library, that requires advances meshing with CUBIT.

2011 - Quarter 2

PI: New approach to higher-order implicit time integration devised We developed a new algorithm that makes it possible to incorporate easily any Runge-Kutta method into finite element, finite difference or finite volume codes for the solution of time-dependent partial differential equations (PDE) and multi-physics PDE systems. This includes any low-order or high-order, explicit / diagonally implicit / fully implicit Ringe-Kutta methods, which are entered in the form of the corresponding Butcher's table. The user / developer only needs to perform the discretization of the stationary residual of the PDE or PDE system. This algorithm was challenging to develop and implement, and so far it works in a simplified version. It will be further developed, optimized, refined and tested in the second quarter of 2011.

PI: Implementation of space-time adaptive hp-FEM for incompressible Navier-Stokes equations started. In exact agreement with the project description, we started to implement adaptive hp-FEM with dynamically changing meshes for incompressible Navier-Stokes equations. We have the option to use continuous elements of up to order 10 for the velocity, and either continuous or discontinuous elements up to order 10 for pressure. Development will continue in the second quarter of 2011. PI: Implementation of space-time adaptive hp-DG method for compressible Euler equations started. We started the development of space-time adaptive higher-order Discontinuous Galerkin (hp-DG) methods for compressible flows. As in the previous item, the target application is coolant flow. While DG methods are usually used together with explicit time integration, we want to use implicit methods because they are much better suited for combination with adaptive meshes (where the CFL condition is a huge problem due to vastly varying element sizes). Development will continue in the second quarter of 2011. Co-PI: Benchmark for coupled neutronics/heat conduction improved The time-dependent benchmark example dealing with coupled neutronics/heat conduction simulations and their verification was extended to account for solutions with greater spatial variations. A preliminary presentation of this work was done at the ANS winter meeting, (November 2010, Las Vegas) and an extended version was submitted as a paper to the upcoming international conference on Mathematics and Computations, sponsored by the ANS and to be held in May 2011. Co-PI: SDIRK-22 method and SDIRK-33 method implemented. SDIRK22 (2 stages, 2nd order) and SDIRK33 (3 stages, 3rd order) methods were implemented by extracting the time-derivative contributions from the residual form and the Jacobian form. An implementation, too complex, has been attempted for any Butcher Tableau specification. Recently, the PI team has devised a simpler and more elegant manner to carry this action out and we will adopt their approach in the future. PI and Co-PI: Setup a new 2D nonlinear radiation-diffusion problem. A 2D nonlinear radiation-diffusion problem was set up in both the PI's and the coPI's multiphysics platforms. Such problems are extremely nonlinear and can serve a stress problems for the methods we develop. Co-PI: Modeling of a 2D fuel pellet A 2D fuel pellet is being modeled. The modeled physical phenomena are: oxygen stochiometry coupled and heat conduction. Diffusion of oxygen includes Fickian and Soret (temperature gradient) terms whereas fuel conductivity depends on temperature and stochiometry. Co-PI: Developing 2D and 3D multigroup reactor simulations. An undergraduate student, Mr. Kevin Dugan, has joined the Co-PI's group and is working on developing 2D and 3D multigroup reactor simulations (neutronics eigenproblems have already been completed in 2D). PI: Investigation of a new adaptive hp-FEM method for eigenproblems with repeated eigenvalues. We performed a thorough literature search and found that there are virtually no adaptive computational methods for eigenproblems that would deal efficiently with repeated eigenvalues. At the same time, repeated eigenvalues are a real concern in nuclear reactor configurations because of their symmetries. The basic problem here is that whenever an eigenvalues is repeated, the eigensolver can (and will) return arbitrary linear combinations of the corresponding eigenvectors. Therefore we are developing a method that will only call the eigensolver one time at the beginning of the computation, and then the desired eigenvalues and eigenfunctions will be resolved with better accuracy using an adaptive algorithm that does not solve the eigenproblem anymore. Two approaches are studied, based on the Newton's and Picard's methods. Co-PI: Published an article about adaptive hp-FEM for the SP3 equations. The Co-PI published an article in Transport Theory and Statistical Physics on the use of hp-FEM for the SP3 equations. PI: Article on Spatial Coupling of Reactor Thermal and Neutron Diffusion Calculations appeared in JCP Exact reference: L. Dubcova, P. Solin, G. Hansen, H. Park: Comparison of Multimesh hp-FEM to Interpolation and Projection Methods for Spatial Coupling of Reactor Thermal and Neutron Diffusion Calculations, J. Comput. Phys. 230 (2011) 1182-1197. PI: Article with new benchmark problems for adaptive hp-FEM accepted to Appl. Math. Comput. Exact reference to the paper is: P. Solin, O. Certik, L. Korous: Three Anisotropic Benchmarks for Adaptive Finite Element Methods, Appl. Math. Comput., accepted in December 2010.

2011 - Quarter 3

PI: New approach to higher-order implicit time integration devised We developed a new algorithm that makes it possible to incorporate easily any Runge-Kutta method into finite element, finite difference or finite volume codes for the solution of time-dependent partial differential equations (PDE) and multi-physics PDE systems. This includes any low-order or high-order, explicit / diagonally implicit / fully implicit Ringe-Kutta methods, which are entered in the form of the corresponding Butcher's table. The user / developer only needs to perform the discretization of the stationary residual of the PDE or PDE system. This algorithm was challenging to develop and implement, and so far it works in a simplified version. It will be further developed, optimized, refined and tested in the second quarter of 2011. PI: Implementation of space-time adaptive hp-FEM for incompressible Navier-Stokes equations started. 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The Co-PI published an article in Transport Theory and Statistical PI: New model of nonstationary coolant flow created and coupled with temperature We finished implementing space-time adaptive higher-order finite element discretization of incompressible Navier-Stokes equations to be used as coolant flow model in multiphysics simulations. The model works nicely and it will be extended to a compressible flow model, and coupled with nonlinear heat conduction and oxygen diffusion. Coupling with heat conduction is in progress. PI: Implementation of space-time adaptive hp-DG method for compressible Euler equations continued We continued work on higher-order Discontinuous Galerkin (DG) discretization of compressible flow equations. Implicit time discretization was implemented and Trilinos NOX package was used to solve the arising nonlinear equation systems. We also implemented a semilinear discretization of the equations to be used as a step towards full Newton method. We noticed that the implicit time discretization combined with a nonlinear solver leads to more significant oscillations (undershoots and overshoots) in the DG than explicit time stepping. We are in contact with several DG experts as well as with people who are skilled in using the Trilinos NOX package, to explain this behavior. PI: Coupling of hp-DG and hp-FEM for multiphysics flow problems started We continued working on a new multimesh discretization technique that makes it possible to solve the flow part of a multiphysics problem with DG and other parts (heat transfer, oxygen diffusion) with continuous higher-order FEM. Significant progress was made and we are going to present it at the FEMTEC 2011 conference. PI: Plug-and-Play software architecture redesigned An important objective of this project is to deliver a plug-and-play software architecture for multiphysics simulations. Due to increasing complexity of multiphysics simulations that are done with the Hermes library, we found it necessary to make significant improvements to its software architecture. In particular, global variables used in weak forms turned out to hinder expansion of multiphysics capabilities of the library and interfacing with solver packages such as Trilinos. Therefore a completely new object-oriented structure of weak forms was designed. Weak forms now have a clean hierarchic structure. Many default weak forms are provided ranging from the Laplace and Poisson equations, one-group and multi-group neutronics, to incompressible and compressible flows. Physical processes can be combined into multiphysics simulations easily. We also improved handling of nonlinearities via cubic splines. Extension of linear problems into nonlinear ones is now a matter of just supplying a spline instead of a constant parameter. Because of a large number of examples that accompany the Hermes library, we will need part of the next quarter to finalize these changes. The tutorial will be updated as well. Co-PI: Progress on coupled neutronics/heat conduction simulations The time-dependent benchmark example dealing with coupled neutronics/heat conduction simulations and their verification was extended to account for solutions with greater spatial variations. A paper has been accepted for presentation at the international conference on Mathematics and Computations, sponsored by the ANS and to be held in May 2011 (paper attached). Co-PI: Work on a coupled oxygen diffusion / heat transfer / mechanical model started A 2D rz and 3D xyz cylindrical model of a fuel pellet is under way. The modeled physical phenomena are: oxygen stochiometry, heat conduction, and thermal stress (only linear elasticity so far). Diffusion of oxygen includes Fickian and Soret (temperature gradient) terms whereas fuel conductivity depends on temperature and stochiometry. In the second half of this quarter, we have started implementing thermomechanical contact (between the fuel pellet and the cladding). Contact is achieved using a Lagrangian formulation and is enforced using an active set formalism. Co-PI: Continued work on 2D and 3D multigroup reactor simulations The undergraduate student who joined the Co-PI's group earlier this year has continued working on developing 2D and 3D multigroup reactor simulations (neutronics eigenproblems have already been completely in 2D and were prese

2011 - Quarter 4

PI: Improvement of adaptive algorithms for transient problems, submission of paper. While finalizing a paper "Adaptive Higher-Order Finite Element Methods for Transient PDE problems Based on Embedded Higher-Order Implicit Runge-Kutta Methods", we realized that the method can be still substantially improved. This was done and now we are able to combine an arbitrary adaptive higher-order spatial discretization with any embedded implicit higher-order Runge-Kutta method in time. This accomplished our task of creating a plug-and-play software architecture of adaptive higher-order methods for time-dependent PDE problems. The paper has been submitted to J. Comp. Phys. PI: Coupling of hp-DG and hp-FEM for multiphysics flow problems continued We continued working on a new multimesh discretization technique that makes it possible to solve the flow part of a multiphysics problem with DG and other parts (heat transfer, oxygen diffusion) with continuous higher-order FEM. Many technical improvements of the methodology were done, and it was presented at the international conference FEMTEC 2011.

PI: New benchmark problem for space-time adaptive methods created. We created a new time-dependent benchmark problem with known exact solution that contains a moving front of arbitrary steepness. This benchmark can be used to test the performance of adaptive methods with dynamically-changing meshes for time-dependent problems. We used the benchmark to demonstrate that our adaptive higher-order methods are by several orders of magnitude faster than standard adaptive low-order methods. PI: Introducing new students, Jordan Blocher and Mateusz Paprocki, to the project. During this quarter, the PI spent significant amount of time with teaching the new students Jordan Blocher (undergraduate) and Mateusz Paprocki (graduate) the finite element method and basic equations relevant for the reactor core. PI: Code cleaning and preparation for first release started. The open source library Hermes (http://hpfem.org/hermes) contains many features that make it attractive to users of commercial softwares such as Comsol or Ansys. As examples we can mention mature adaptive hp-FEM algorithms, monolithic multimesh discretization of multiphysics coupled problems, adaptivity with dynamical meshes for transient problems, or a database of over 30 time-integration methods including 7 embedded implicit higher-order methods for temporal adaptivity. Due to the constantly increasing demand, we decided to clean the code and prepare it for an official release, that will be followed with creation of an Ubuntu package. This requires a large amount of work that is not visible now, but it will facilitate the development of adaptive higher-order methods for multiphysics reactor problems in the future. PI: Continued work on fully implicit higher-order DG methods for coolant flow. We made progress in the application of the Jacobian-Free Newton-Krylov (JFNK) method to nonstationary compressible coolant flow. The Trilinos NOX solver already works, but we are getting spurious oscillations at steep gradients. Currently we are in the middle of implementing suitable slope limiters that will take care of this problem. PI: Several presentations of the computational methods developed in this project. The results of the projects were presented at the international conference FEMTEC 2011 (South Lake Tahoe, May 9 - 13, 2011) and at the University of Erlangen-Nuernberg, Germany. The PI held a series of six lectures at the University Roma Tre (Italy) about adaptive higher-order discretizations of multiphysics problems. PI: Comparison of the Hermes library with DealII The open source library DealII is older and more widespread than the Hermes library developed by our group. We used an adaptivity benchmark with known exact solution to compare the performance of these two libraries. Hermes was much better that DealII when automatic hp-adaptivity was used. This is not so surprizing since adaptive hp-FEM is a strength of Hermes. But Hermes was also much better when low-order adaptive h-FEM was used. This was a bit surprizing. Although the problem had symmetries, DealII produced meshes that were non-symmetric. These comparisons will be published online.

Co-PI: Progress on time-dependent benchmark problem. The time-dependent benchmark case dealing with coupled neutronics/heat conduction simulations and their verification was extended to account for solutions with greater spatial variations. The paper has been presented at the international conference on Mathematics and Computations (May 2011), sponsored by the ANS. The paper was already attached to the previous quarterly report. This paper has been selected for a full journal publication in Nuclear Science and Engineering. In its current state, the benchmark only includes manufactured soluti o-PI: Thermo-mechanical modeling of a nuclear fuel pellet. Work has continued regarding the thermo-mechanical modeling of a nuclear fuel pellet. Both 2D rz and 3D xyz cylindrical models are being employed. This quarter, we have implemented a contact algorithm (wrapped around the nonlinear Newton solve) to determine the portion of the fuel/clad interface where contact is established. Contact modeling is achieved using a Lagrangian formulation and is enforced using an active set formalism. An abstract has been submitted to the ANS Winter Meeting, Nov. 2011) and is attached. Acceptance decision is expected next month. Co-PI: Internship for a PhD student. Damien Lebrun-Grandie, PhD student sponsored under this grant, is interning at the ORNL, working with the multiphysics fuel modeling team this summer.

Co-PI: Modeling time-dependent monophasic fluid flows. Work has also begun to model time-dependent monophasic fluid flows in 2D using implicit time integrators (and thus solving the resulting nonlinear problem with a Newton-based approach). Standard test cases (lid-drive cavity, and shock tube) has been successfully tested. Code implementation was verified using manufactured solutions.

Thermo-mechanical modeling of a nuclear fuel pellet In year 2, work was initiated (and continued during the fourth quarter) regarding the thermo-mechanical modeling of a nuclear fuel pellet. Both 3D rz (axi-symmetric) and 2/3D xy/xyz models are have been developed. The equations solved so far are the heat conduction coupled with mechanical displacement. A thermal strain component of the strain tensor couples the temperature field to the displacement field. In return, the geometrical modifications influence the thermal solution. This multiphysics applications is solved in a monolithic fashion with a Newton-Krylov solve. Furthermore, we have implemented a contact algorithm (wrapped around the nonlinear Newton solve) to determine the portion of the fuel/clad interface where contact is established. Contact modeling is achieved using a Lagrangian formulation and is enforced using an active set formalism to determine the mesh interfaces that are in contact. Two conference proceedings have already resulted from this ongoing work. Extension of multiphysics verification code In year 2, a multiphysics code verification exercise for coupled time-dependent neutronics/heat conduction was extended to account for solutions with greater spatial variations. The resulting work was presented at the international conference on Mathematics and Computations (May 2011), sponsored by the ANS. This paper has been selected for a full journal publication in Nuclear Science and Engineering. In its current state, the benchmark only includes manufactured solutions which are employed for code and algorithm verifications. A realistic rod ejection problem is being modeled for the journal publication. Implicit solvers for monophasic flows In year 2, work was initiated to model time-dependent monophasic fluid flows in 2D using implicit time integrators (and thus solving the resulting nonlinear problem with a Newton-based approach). Standard test cases (lid-drive cavity, and shock tube) has been successfully tested. Code implementation was verified using manufactured solutions. Recently, work begun on two-phase flow simulations. Employing a Discontinuous FEM (DG) approach requires that numerical flux quantities (of mass/momentum/energy) be computed at each interface of the mesh. For instance, in the R7 project of INL (new reactor safety code), the standard Rusanov numerical flux is employed with the eigenspectrum of the Euler equations for the fluid mixture (liquid+vapor). We demonstrated that the resulting eigenvalues for 4-, 5-, and 6-equation two-phase fluid models cannot be approximated at the ones from Eulers equations for the mixture. Therefore, our approach shows the promise for a more rigorous approach for DG numerical fluxes in two-phase flow simulations. Outreach Damien Lebrun-Grandie, PhD student sponsored under this grant, interned at the ORNL, working with the multiphysics fuel modeling team in summer 2011. Collaboration with ORNL staff The PI P. Solin started collaborating with V. de Almeida (ORNL) on the simulation of radiative heat transfer in nuclear waste. This collaboration is mentioned here because it leverages the multiphysics higher-order finite element library Hermes that is being developed in this project. Based on the promising preliminary results, Dr. Solin and Dr. de Almeida submitted a preproposal to the NEUP program together. Enabling mulphysics models with different fields defined in different spatial domains Major implementation effort was dedicated to extend the multiphysics library Hermes to solve multiphysics problems where not all physical fields are defined in the same domain. For example, in coupled neutronics-thermal-flow problems, the flow domain is different from the domains where the temperature and neutronics are solved. The new functionality was highly nontrivial to implement but it is ready. It was used to solve a model problem combining heat transfer and flow. More advanced problems combining neutronics-thermal-flow, and others, will be solved in Year 3.

2012 - Quarter 1

PI: Improvement of adaptive algorithms for transient problems, submission of paper. While finalizing a paper "Adaptive Higher-Order Finite Element Methods for Transient PDE problems Based on Embedded Higher-Order Implicit Runge-Kutta Methods", we realized that the method can be still substantially improved. This was done and now we are able to combine an arbitrary adaptive higher-order spatial discretization with any embedded implicit higher-order Runge-Kutta method in time. This accomplished our task of creating a plug-and-play software architecture of adaptive higher-order methods for time-dependent PDE problems. The paper has been submitted to J. Comp. Phys. PI: Coupling of hp-DG and hp-FEM for multiphysics flow problems continued We continued working on a new multimesh discretization technique that makes it possible to solve the flow part of a multiphysics problem with DG and other parts (heat transfer, oxygen diffusion) with continuous higher-order FEM. Many technical improvements of the methodology were done, and it was presented at the international conference FEMTEC 2011.

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2012 - Quarter 2

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2012 - Quarter 3

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Developing DG numerical fluxes for two-phase flow simulations In this quarter, work was initiated in year 2 and pertaining time-dependent monophasic fluid flows in 2D using implicit time integrators is continued. Standard test cases (lid-drive cavity, and shock tube) has been successfully tested and code implementation was verified using manufactured solutions. We are now extending this preliminary to the situtations of low-Mach flows (representative of realistic reactor applications). In addition, work also begun on two-phase flow simulations. Employing a Discontinuous FEM (DG) approach requires that numerical flux quantities (of mass/momentum/energy) be computed at each interface of the mesh. For instance, in the R7 project of INL (new reactor safety code), the standard Rusanov numerical flux is employed with the eigenspectrum of the Euler equations for the fluid mixture (liquid+vapor). We demonstrated that the resulting eigenvalues for 4-, 5-, and 6-equation two-phase fluid models cannot be approximated at the ones from Eulers equations for the mixture. Therefore, our approach shows the promise for a more rigorous approach for DG numerical fluxes in two-phase flow simulations. We will seek demonstration of this capability for 1D two-phase flows this quarter. Refactoring the Hermes3D library started During Years 1 and 2, the work on the 3D version of the Hermes library was stopped according to the plan, and we worked only on the 2D version. As a result, the 2D version of the library was significantly advanced. It features adaptive multimesh hp-FEM for time-dependent multiphysics problems, novel paradigm for time-integration based on arbitrary Butcher's tables, multithreading on the level of assembling, among others. At the beginning of October 2011, the structure Hermes3D library was nowhere close to Hermes2D. Therefore, we started a tedious process of adjusting the structure of the 3D library to correspond to the 2D one. This is necessary in order to port the above mentioned methods from the 2D code to the 3D one. The refactoring has progressed significantly during the 1st quarter of 2012 and it will be finished in the second quarter. This is in good agreement with the goals for Year 3.

Finalizing and testing a new combined space-time adaptive monolithic hp-DG / hp-FEM method for multiphysics coupled problems The hp-DG method is a great discretization method for flow problems including coolant flow. For other types of problems such as neutronics or heat conduction this method is significantly more computationally expensive compared to hp-FEM, and it does not bring any remarkable advantages. Therefore approximately a year ago we started the development of a combined hp-DG / hp-FEM method where the former is applied to the flow equations of the multiphysics problem, and the latter to the remaining equations. It is worth mentioning that this method very naturally fits into the plug-and play software architecture developed in this project. The resulting discretization is monolithic and it inherits all advantages of the original multimesh hp-FEM method that was developed earlier in this project. In particular, various components of the multiphysics problem are discretized on different meshes that undergo individual adaptivity mechanisms. The resulting discretization is monolithic (there is no operator splitting of any kind) so the complete physics is preserved on the discrete level. And last, one can perform time integration using an arbitrary Runge-Kutta method (explicit or implicit, low-order or high-order). A concrete Runge-Kutta method is the input parameter for the simulation via its Butcher's table. The method was presented by Lukas Korous at the SCA 2012 conference in Las Vegas in April 2012 (presentation has 30 MB and could not be uploaded, but we at least attached the screenshot of first two slides with the title page and acknowledgment). P. Solin presented at the same conference new results on incorporating arbitrary-high embedded time integration methods into multiphysics coupled problems (presentation attached). Invited presentation at UNLV P. Solin was invited to UNLV to present adaptive hp-FEM methods implemented in the Hermes library. Presentation is attached. Work on a new adaptive hp-FEM method for eigenproblems was finished and paper submitted Approximately a year ago we started working on a new adaptive hp-FEM method for eigenproblems whose significant advantage is that it works reliably also for repeated eigenvalues. The method calculates a coarse mesh approximation and then it employs an adaptive algorithm based on the Newton's method to pursue the concrete eigenfunction, without switching to other eigenfunctions that may exist for the same eigenvalue. In this quarter we finished all numerical experiments, finalized the paper, and submitted it to Journal of Applied and Computational Mathematics. (paper attached). Refactoring of Hermes3D library finished The refactoring of the Hermes3D library has started in the first quarter of Year 3 as we described in the previous quarterly report. It has progressed significantly during the 1st quarter of 2012 and was finished according to the plan in the second quarter. Now the algorithmic and software foundation of the Hermes2D and Hermes3D libraries converged, although the former is still a lot more developed compared to the latter. This allowed us to begin the process of generalization of the novel algorithms that we developed in Years 1 and 2, to 3D.

Progressing towards the main goal of Year 3 In the original proposal, we promised to deliver the following at the end of Year 3: "At the end of the third year, we will demonstrate that the 3D library can solve coupled problems of neutronics/conduction using space-time adaptive hp-FEM." Therefore, after finishing the refactoring of the Hermes3D library to be compatible with Hermes2D, we started to work on 3D extension of the fundamental 2D algorithms from Hermes2D that are needed for this. The major component that needs to be generalized to 3D is the multimesh hp-FEM discretization technology. We started working on it, and as expected, the 3D implementation is much more involved than the 2D one. Once the multimesh hp-FEM is ready, the space-time adaptivity with synamical meshes will not take so much effort, but this step requires a significant amount of work. We estimate to work on it for the entire Quarter 3, and finish it in August 2012. This will be in time to deliver objectives of Year 3 as promised.

2012 - Quarter 4

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Continued work on combined adaptive monolithic multimesh hp-FEM/hp-DG method In this quarter we finalized and cleaned up algorithms for the combined adaptive monolithic hp-FEM/hp-DG method for multiphysics coupled problems, that we developed during the last year. Representative results were obtained and a paper is in preparation. The paper will be submitted during the next quarter. Continued work on the 3D solver The 3D code is already capable of automatic hp-adaptivity and we are preparing it for the implementation of the monolithic multimesh hp-FEM discretization which is a necessary prerequisite for space-time adaptivity with dynamical meshes. However, compared to the 2D code, the work on the 3D code is much more time consuming. The assembling is much slower than in 2D. We profiled the code and found that the most time-consuming operation is higher-order numerical quadrature. Its computational complexity is O(p^3) where p is the polynomial degree of the element. We have thoroughly revised numerical quadrature in Hermes3D and improved the representation of higher-order shape functions. This reduced the assembling time to approx. 50

Subcontract with the Co-PI was terminated The Co-PI failed regularly to provide his portion of data for the quarterly reports. Without the PI's approval, in the third year he started to use the NEUP funds to work on his projects that were not in the scope of the present project. This is evident from his last reports as well as from his final report that is attached. Example such projects are contact problems and supersonic compressible flow. Based on our request, the present project was extended until December 31, 2012. Continued work on issues that the Co-PI failed to deliver The Co-PI failed to implement Jacobian-free Newton-Krylov methods in the Hermes library, and compare them with the standard Newton's method, as was his task according to the project description. We finished implementation of JFNK for 2D problems and started implementation for 3D problems. Continued work on extending the multimesh hp-FEM discretization from 2D to 3D This includes more work than was expected - the 3D setting contains not only all problems from 2D but also qualitatively new problems that need to be overcome. For example, in the technique of arbitrary-level hanging nodes we have not only constraints by edge functions as in 2D, but also by face functions, and these constraints propagate through the hp-FEM mesh in new ways not seen in

A Scope of the Proposed Work

To change the paradigm for multiphysics simulations in reactor design & analysis:

Many of the physical phenomena occurring in nuclear reactors, under normal or accidental situations, are inherently tightly coupled – for example neutronics/thermal-hydraulics or fuel pellet thermo-mechanics, ... Furthermore, the length and time scales of the various physics components may greatly vary and evolve during a transient. Yet, most of the algorithms employed today to solve such complex physical phenomena (1) rely on simple data exchanges in between mono-disciplinary codes and (2) employ fixed grids in space and time. The current approach presents two serious drawbacks. First, it is now well established that not resolving the nonlinearities in between coupled physics can lead to a loss of accuracy and even stability in the numerical simulations [24]. Second, the lack of space-time adaptive meshes may prevent the accurate resolution of relevant physical phenomena, or worse, may ignore localized features. These two drawbacks are significant impediments to a science-based approach for the accurate simulation and prediction of nuclear system behaviors. In this project, we propose to address both obstacles, the consistency of the nonlinear simulation and the accuracy of the spatio-temporal discretization, by developing a novel mathematical methodology and the associated algorithmic framework and software architecture. The space-time adaptive high-order monolithic discretization of nonlinear time-dependent multiphysics equations proposed here will be employed to address some representative challenges arising in the modeling of nuclear systems: coupled neutronics/thermal-hydraulics, thermal stress and oxygen diffusion in UOX fuel pellets. This technique will make it possible to

1. Employ high-order spatially adaptive discretizations (possibly different for each physical field if the fields exhibit significantly different phenomena or different spatial scales [22]).

2. Use high-order automatically adaptive implicit time stepping schemes (also possibly different for each field in the case of multiple time scales).

3. Discretize arbitrary combinations of nonlinearly-coupled physics in a monolithic fashion [23] via standard Newton as well as Jacobian-Free Newton-Krylov (JFNK) methods [24, 25]. We will investigate systematically various types of preconditioners for the JFNK methods for several multiphysics situations, and perform a systematic comparison of JFNK methods with standard Newton methods for these problems.

It is important to note that a significant amount of the "machinery" has already been developed by the PI and Co-PI over several years, making the proposal goals well within reach. Such a level of sophistication would not be reasonable nor feasible starting from scratch.

In the following sections, we provide details on the numerical methods (the space, time, and space-time adaptivity techniques, and the tightly coupled resolution of multiphysics problems with their efficient preconditioning), and describe in detail the logical path to the accomplishments of the project goals listed above. The software packages/libraries developed by the PI and Co-PI will play an essential role in the proposed research, and therefore their main capabilities are described briefly in the "Capabilities" document.

B Numerical Methods

B.1 *hp*-FEM Spatial Adaptivity

The spatial discretization of the underlying governing equations will be carried out using *hp*-adaptive higher-order finite element methods (*hp*-FEM). These methods have been developed and used for the last 20+ years [20] but remained for quite some time the purview of the mathematics community and were tested on simple problems of marginal engineering interest. Nonetheless, over the last decade, these methods have enjoyed significant practical developments and are now commonly used for realistic engineering applications by the structural mechanics and electromagnetics communities [21]. These methods are unique by their extremely fast, exponential convergence that makes them vastly superior to standard low-order FEM and standard h adaptive FEM [21], but they have received little interest in nuclear engineering so far (with the exception of [27]).

Such spectacular rates are possible due the competitive choice of refinements between h adaptivity, or mesh subdivision (adequate for regions where the solution is not smooth), and p adaptivity, or polynomial order increase (adequate for smooth regions). A highly sophisticated, engineering-grade *hp*-FEM software library developed by the PI's group over the last 6+ years will be employed in the course of this work to devise spatially adapted meshes.

B.2 Temporal Adaptivity

Tackling the nonlinear system of equations as a whole, rather than employing an operator-splitting (OS) approach allows to tap into the accumulated knowledge for integrating implicitly in time nonlinear equations using (generalized) Implicit Runge Kutta (IRK) methods. In IRK methods, the following nonlinear system is solved $u' = f(t, u)$ where u represents a dependent variable (from any physics component). Using the general formalism of IRK methods developed by Butcher et al., this system of equations can be implicitly integrated in time with high-order of accuracy. Implicit time integration is required due to the large spread of time scales, resulting in very stiff nonlinear system of equations. As with more pedestrian explicit Runge-Kutta methods, IRK methods also exist as embedded pairs, where the same intermediate solution stages can be used to yield a lower order solution; the difference between the high and low order answers give a computationally inexpensive error estimate which can be effectively employed to control the temporal discretization error and, therefore, selectively adapt the time step size. Each stage of the IRK method requires the resolution of the nonlinear system of equations. This is accomplished through a Newton-type method, in which the expensive Jacobian matrix $\partial f/\partial u$ can be cleverly omitted. This approach, called Jacobian-Free Newton-Krylov (JFNK) method, is now increasingly popular due the work of D. Knoll and collaborators [24], and other groups. The application of JFNK to our specific problems will be discussed in Paragraph B.4.

B.3 Spatio-Temporal *hp*-Adaptivity with Dynamical Meshes

Novel space-time adaptive higher-order methods: Nowadays, space-time adaptive finite element methods with dynamical meshes are still used rather scarcely, and only for simpler problems (single physics such as parabolic) and in the context of standard low-order FEM. The PI's research group is the only one solving realistic time-dependent nonlinear multiphysics coupled problems using space-time adaptive *hp*-FEM on dynamical meshes. The method is based on a combination of the novel multimesh *hp*-FEM [22, 23] combined with the classical Rothe's method. Note that the meshes for the velocity and pressure are different. In reality, they also evolve in time independently of each other. *In spite of that, the discretization is monolithic and no operator splitting is involved.*

The novel method can capture extremely accurately flow artifacts across vastly different scales, which would be plain impossible using methods based on fixed meshes. Preliminary work [22, 23] has demonstrated that the space-time adaptivity can improve the accuracy and efficiency of the simulation of time-dependent problems dramatically.

Another example is related to the multiphysics problem of heat and moisture transfer in the solid walls of a PWR nuclear reactor (simplified axisymmetric geometry). Here, the temperature evolves on a very different temporal scale than the moisture, and so each field is discretized on an individual higher-order finite element mesh that changes dynamically in time.

B.4 Tight Coupling Scheme for Multiphysics Simulations

Multiphysics framework based on Newton/JFNK techniques:

Traditional coupling paradigms rely on solving the different physics in a loosely coupled fashion, a technique mathematically described as operator-splitting (OS), where the output of one code is passed as input to another. The major drawback of this approach is reduced accuracy and stability of the simulations [18, 19], originating in the fact that coupling terms in between the various physics components are dealt with inconsistently. In order to fully resolve the nonlinearities between the various physics components, a tight coupling approach must be employed. This generally calls for re-formulating the system of equations from a paradigm based on a "juxtaposition" of monodisciplinary physics to a single nonlinear problem, whose solution is to be obtained using Newton's method. Such a change in the coupling strategy is far from appealing, as many man-years of mono-disciplinary code development verification and validation could be lost; furthermore, such a monolithic code could be more complicated to develop and maintain. Fortunately, over the past decade, Jacobian-free Newton-Krylov (JFNK) methods for multiphysics applications have significantly mature [24, 25, 28]. With JFNK methods, the distinction among the various physics is easily retained and the number of coupled physics can be easily changed and tuned to the specificities of a given problem, yet a tightly coupled solution is obtained. One may think of such methods as performing a tightly coupled simulation using a loosely coupled software architecture. In the next paragraph, we describe some of the technology associated with JFNK and present our current software framework which will host the developments proposed in this research.

After spatial discretization and implicit time integration, the nonlinear governing laws describing the multiphysics problem can be viewed as a nonlinear system $F(u) = 0$ where u represents the independent variables (from all physics component). This nonlinear residual F is built "physics by physics"; for a brief illustrative example, considering two physics A and B; the independent variables would be described as $u = [u_A,\ u_B]^T$ and the nonlinear residual as $F = [F_A(u),\ F_B(u)]^T$; The portion of the nonlinear residual $F_A(u)$ of physics A can be built by passing the subset of u that is needed in physics A. In such a fashion, a multiphysics driver code can manage an arbitrary number of separate physics components. Our current driver relies on world-class open source libraries, such as `PETSc` for linear and nonlinear solvers (including JFNK), `libmesh` for the Finite Element discretization of various PDEs, and `gmsh` & `ParMetis` for mesh generation and parallel domain decomposition. The multiphysics platform operates on single-processor desktop machines as well as parallel clusters. We have already validated our approach for various prototypic coupled multiphysics situations.

Novel monolithic high-order discretization method for multiphysics problems: In contrast to the widely used operator-splitting (OS) methods (see, e.g., [18, 19] and the references therein), we propose a novel monolithic approach that preserves exactly the coupling structure of the multiphysics coupled problems from the continuous to the discrete level. The method is based on a novel adaptive multimesh *hp*-FEM discretization technique [22, 23].

Part A represents the *master mesh*. This is a very coarse initial mesh, for example one element which spans the entire domain. The master mesh is not used for discretization normally, but it forms the top of a tree-like structure of meshes for all physical fields or solution components in the system. These meshes are obtained from the master mesh through mutually independent series of refinements. Part E shows the *union mesh* which obtained as a geometrical union of all elements in all meshes in the system (imagine printing all meshes on transparencies and putting them over each other). The union mesh is virtual (not constructed in the computer memory physically), but its elements are parsed by the multimesh assembling algorithm to build the global stiffness matrix for the multiphysics problem. Besides this, the multimesh assembling algorithm works analogously to the standard assembling algorithm in (single-mesh) *hp*-FEM.

The tree-like structure of meshes allows us to *access all physical fields at any given integration point simultaneously*. This means that there is no error caused by transfer of approximations between different meshes which is characteristic for most operator splitting (OS) methods [18]. This error is known to affect not only the accuracy, *but also the stability of OS schemes* [19]. Another major problem in OS methods is the error caused by incomplete iteration. By preserving the coupling structure between the continuous and discrete levels, our method avoids this error completely, and thus provides a better framework for sensitivity and uncertainty analysis than existing operator splitting methods.

C Novel "Plug-and-Play" Algorithmic and Software Platform

Plug-and-play architecture for numerical methods: For several years, both the PI and Co-PI have been developing independently of each other numerical methods and software libraries for multiphysics problems aimed at high-fidelity tightly coupled multiphysics simulations. The PI has been putting more emphasis on adaptive higher-order finite element methods (*hp*-FEM) combined with standard Newton's methods while the Co-PI concentrated on JFNK methods, preconditioners, and implicit adaptive higher-order time-integration methods. In this project, the PI and the Co-PI will create a common modular software platform that will make it possible to exchange data and algorithms easily, as well as add modules with new numerical methods. The proposed project brings together two key groups to investigate Newton and JFNK methods combined with novel high-order space-time adaptive monolithic discretization algorithms for multiphysics problems in nuclear engineering, and develop for the DOE a unique expertise in science-based high-fidelity multiphysics simulations. This will make it possible to create quickly arbitrary multiphysics models and solve them with various numerical methods. The novel platform will be used to compare the performance of Newton and JFNK methods for several multiphysics problems in nuclear engineering, test various preconditioners for JFNK, study the performance of JFNK methods combined with space-time adaptive methods, etc.

Plug-and-play "assembly" of multiphysics problems: Both the software libraries of the PI and Co-PI allow for a simple plug-and-play "assembly" of arbitrary multiphysics problems via predefined linear and bilinear forms. This is done using a relatively small number of predefined linear and bilinear forms such as `int_u_v(...)` for reaction terms, `int_dudx_dvdx(...)` for diffusion terms, etc. The software of the PI moreover allows to use multiple element types in one computation, such as the standard continuous H^1-elements for the temperature, velocity and other quantities, vector-valued "edge elements" for the electrical field, vector-valued "face elements" for the magnetic field, and discontinuous L^2-elements for the pressure (in some applications). The software of the Co-PI possesses equivalent features: flexibility of coupling various physics components, state-of-the-art FEM library package, but focused their efforts on JFNK framework and parallel implementation rather than high-order spatial discretization.

D Project Management Plan

D.1 Preliminary results of the PI and the Co-PI

To span in three years all the different problems described above is a exciting goal, but both the PI and the Co-PI will leverage a number of previous results and capabilities. In both cases, these are not only theoretical results but mainly novel numerical methods, algorithms, and software libraries developed during the last several years.

The PI has 10+ years of experience with higher-order methods and automatic adaptivity, including space-time adaptivity for various types of multiphysics problems such as thermoelasticity, flame propagation, thermally-conductive incompressible flow, two-phase flow, compressible inviscid flow, electromagnetic-thermal problems and others. Some of these results have been already published in journals and the most recent ones have been presented at international conferences such as FEMTEC 2009 or SIAM CSE meeting 2009.

The Co-PI has many preliminary results and his own software library for implicit higher-order time-discretization schemes, JFNK methods, and the simulation of various multiphysics processes such as reactor transients multigroup diffusion and

S_N transport, and others.

D.2 Logical Path to Accomplishing Scope, Description of Tasks & Schedule

It is essential for the success of this project that the investigators create soon a first working version of a common algorithmic and software platform which is sufficiently modular to allow for the plug-and-play operation with various numerical methods described above, including easy interfacing with external numerical packages such as Trilinos or PETSC, visualization packages such as ParaView or GMV, and mesh generation libraries such as Cubit or Gmsh. This new platform will allow us to exchange data and algorithms smoothly, and develop new computational methods efficiently using a joint effort. The platform will be constructed in several logical steps using a series of model problems with increasing level of complexity.

Year 1

Step 1: We will use several lower layers of the PI's software library as the first version of the common software platform for both investigators. The basic platform will be able to read and process meshes, assemble discrete problems, solve them via external packages, perform a-posteriori error estimation via enriched polynomial spaces, perform automatic *hp*-adaptivity, and visualize the results. We will implement a basic time-integration scheme (non-adaptive implicit Euler method) and test the functionality of the platform using nonstationary linear diffusion for neutrons. Next we will add higher-order adaptive implicit higher-order time-integration methods from the Co-PI's code. This task is required since the PI's methods are based on the Rothe's method while the Co-PI's methods are based on the Method of Lines.

Step 2: After the nonstationary linear diffusion for neutrons can be solved using space-time adaptive *hp*-FEM, we will add nonlinear solvers based on the standard Newton's method (from the PI's code) and on JFNK methods (from the Co-PI's code). We will establish an interface that makes it straightforward to switch from one method to another. These methods will be tested on nonlinear heat conduction equation. Last, we will extend the platform via the multimesh *hp*-FEM technique to be able to solve the multiphysics problem consisting of neutron diffusion (with temperature-dependent cross-sections) and nonlinear heat conduction. At the end of the second step, we will be able to solve this coupled problem efficiently and *with controlled accuracy in both space and time* via space-time adaptive multimesh *hp*-FEM.

Internal tests: At the end of every logical step, we will implement internal tests for all important new functionalities. Such tests are standard software engineering practice and they are absolutely essential for the stability of a software system at this level of complexity. Both the PI and the Co-PI have been using this practice for years in their software project.

Year 2

In the second year, the new software platform will be sufficiently mature so that the novel space-time adaptive higher-order finite element methods can be applied to more complicated multiphysics problems. The PI will add new physics describing nonstationary coolant flows. For this, he will leverage existing functionality of his software in stabilized compressible viscous flow models. (Let us remark that stabilization of compressible Navier-Stokes equations discretized by means of higher-order FEM is highly nontrivial – it took several months of work to the PI until he tested the SUPG, Taylor-Galerkin, Least-Squares, and hyper-viscosity approaches and selected the optimal one for the space-time adaptive *hp*-FEM). The Co-PI will employ the new methods to study fuel performance (nonlinear heat conduction + oxygen diffusion). In the second half of year 2, both investigators together will develop a model for coupled neutron diffusion/heat conduction/single phase fluid flow.

Year 3

In the third year, the investigators will use joint effort to extend the 2D methodology and software platform to 3D. This is much more involved than the 2D case, but we will leverage several years of work that has been done on the *hp*-adaptive 3D solver. Currently, the PI's 3D code can solve time-independent problems using adaptive *hp*-FEM on unstructured hexahedral meshes. The extension of the adaptive multimesh *hp*-FEM, which is the main ingredient for the novel space-time adaptive algorithms, will be the main responsibility of the UNR group. Once this is done, the extension of the space-time adaptivity is straightforward. The Co-PI will concentrate on the extension of the JFNK methods and preconditioners from 2D to 3D, interfacing with external libraries, and he will be responsible for the preparation of concrete problems to be solved, including geometries and meshes. At the end of the third year, we will demonstrate that the 3D library can solve coupled problems of neutronics/conduction using space-time adaptive *hp*-FEM.

Although this was not mentioned in the plan for each year explicitly, for every new model we will implement an optimal preconditioner for the Jacobian-Free Newton Krylov (JFNK) method, and compare the performance and feasibility of JFNK with the standard Newton's method in the context of space-time adaptive *hp*-FEM discretizations on dynamical meshes.

D.3 Milestones and Deliverables

We will deliver a new methodology for space-time adaptive high-order monolithic discretization of arbitrary time-dependent multiphysics PDE problems in nuclear engineering. We will also deliver a new software architecture that allows for simple plug-and-play assembly of arbitrary multiphysics PDE systems, and their solution via space-time adaptive higher-order methods on dynamical meshes. Demonstrative examples will include (i) reactor transients, (ii) coupled heat conduction and oxygen diffusion in fuel rods, and (iii) coupled neutron diffusion/heat conduction/single phase fluid flow. The deliverables will include quarterly technical progress reports, an annual report with oral presentation at engaged DOE laboratories (multiphysics group at INL, Simulation-Based High-Efficiency Advanced Reactor Prototyping (SHARP) project at ANL, multiphysics of the Nuclear Science and Technology Division at ORNL).

D.4 Type/Description of Facilities That Will be Used to Execute the Scope

This project only requires high-performance computing (HPC) infrastructure, no experimental facilities or other equipment is needed. Both investigators have access to sufficient HPC capabilities to complete the proposed research. The University of Nevada, Reno has a high-performance computing cluster composed of 118 compute nodes with a total of 386 CPU cores, combined 518 Gigabytes of RAM, and 24 Terabyte NAS. The Texas A&M University possesses a supercomputing facility that includes IBM p5-575 Cluster *Hydra* with 640 computing nodes, 1280 GB memory and a peak performance of 4.1 TFlops, and SGI Altix 3700 Supercomputer *Cosmos* which has 128 cores, 256 GB of memory, and peak performance 666 GFlops.

Substantial prerequisite for the proposed project are the software libraries that both the PI and the Co-PI have been developing for the last several years. While following the same objectives and software engineering practices, their software packages contain complementary technologies that the investigators will merge into a novel, highly flexible plug-and-play software platform for multiphysics problems.

D.5 Roles and Responsibilities of Each Partnering Organization

The group of the PI will contribute with expert knowledge of adaptive higher-order finite element methods (*hp*-FEM), space-time adaptive *hp*-FEM on dynamical meshes, and an existing algorithmic platform suitable for an easy plug-and-play assembly of arbitrary multiphysics problems and their monolithic discretization using adaptive high-order methods combined with the standard Newton's method. The PI will coordinate the efforts will the Co-PI and make sure that all quality assurance (QA) requirements are satisfied and all deliverables accomplished. He will be working closely with the postdoctoral fellow on the design of the new software platform and the novel space-time adaptive *hp*-FEM methods. The PI will also mentor a postdoc and prepare him for an independent research career.

The group of the Co-PI will contribute expert knowledge of multiphysics problems in nuclear engineering, adaptive high-order implicit time stepping methods, Jacobian-free Newton-Krylov methods, preconditioning methods for multiphysics systems, and high-order DG discretization techniques.

The level of complexity of the proposed research requires combining the hiring of one postdoctoral assistant (at the PI's institution) and one PhD candidate to work with the Co-PI. The post-doctoral fellow has been working with the PI for several years. His task will be to help design the software platform where the PI and the Co-PI will work together, actively develop the new computational methods with the PI, and maintain and extend the new software platform as new numerical methods and capabilities are added.

E Relevance to DOE Mission

The proposed research is fully aligned with the DOE mission, work item **AFM-4, Multiphysics Coupling**. The areas for multiphysics coupling algorithms research, critical to DOE, include (a) the development of [at least] second order in time coupling methods and (b) software architecture for efficiently treating the coupled problems.

The numerical techniques to be developed in this project have the potential to significantly increase the efficiency and fidelity in the simulation of multiphysics transients/accidents in complex engineering systems. To our best knowledge, higher-order space-time adaptive finite element discretizations based on dynamically changing meshes have not been investigated systematically for multiphysics problems in nuclear engineering yet.

The novel plug-and-play software architecture is based on state-of-the-art software libraries and it will promote the ability to define new and combine existing physics module implementations to study different phenomena, define and combine different numerical techniques, configure the code easily to run on new platforms, and develop new physics components without expert knowledge of the entire system.

The proposed work addresses both the temporal accuracy (through a Newton/JFNK approach combined with implicit adaptive high-order time-integration methods) and the spatial accuracy (through dynamically-changing adaptive higher-order meshes). The novel methods do not use operator splitting (OS) and *preserve exactly the multiphysics coupling structure from the continuous to the discrete level*, which eliminates the usual accuracy and stability problems of OS methods, and leads to more realistic simulation results.

The project responds to the AFCI need for *science-based approaches for the assessment of performance, reliability, and safety of existing and new nuclear energy systems.* Active collaboration with various multiphysics teams across the DOE complex will be pursued, notably with INL (their Multiphysics team is leading the development of new algorithmic framework for multiphysics problems), ANL (who is spearheading the SHARP project (Simulation-based High-fidelity Advanced

Reactor Prototyping), and ORNL (their multiphysics team is also very active in fuel performance and coupled neutronics/thermal-hydraulics).

Both the postdoc and the graduate student will be trained in the new paradigm of high-fidelity multiphysics simulations and will certainly become an asset for the DOE complex as several national laboratories are actively developing multiphysics capabilities.

F Quality Assurance

The project outcomes will be presented annually at a DoE lab as well as at a national conference. We will publish exclusively in high-impact international journals (ISI journals with impact factor). In addition, we will adhere to all RFP QA procedures, as well as to the ones in place at our institutions. For the purpose of code/software development, the following QA procedures (already in place in each of our software) will be rigorously followed: version control of code, inline documentation, regression test suite (consisting of unit tests, single physics tests, multiphysics tests). Both UNR and TAMU are bound by state laws on some items of the Standard Research Sub-Agreement, and will need the opportunity to negotiate these items.

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