Computer Modeling of Multiphysics Problems

P. Solin, O. Certik, A. Poudel, S. Regmi (UNR Department of Mathematics and Statistics)
D. Pugal, E. Santiago (UNR Department of Mechanical Engineering)
Collaborators: `http://hpfem.org/people`

Computational Challenges

Multiphysics problems are present in the computer modeling of engineering processes that involve the interaction of two or more physical fields. Examples of such processes include:

- **microwave heating** (electric field, temperature),
- **setting of concrete** (chemical reactions, temperature, moisture, deformations),
- **nuclear reactions** (chemical reactions, neutron flux, temperature, flow, deformations).

These problems are typically described by means of nonlinear time-dependent partial differential equations (PDE), and their solutions involve vastly different spatial and/or temporal scales. This behavior poses tremendous challenges to numerical methods. In addition, error analysis mechanisms that work well for linear PDE are not applicable here – multiphysics PDE systems are beyond what modern mathematical analysis can handle.

Adaptive Finite Element Methods

The Finite Element Method (FEM) is the most powerful numerical method to solve partial differential equations (PDE) and multiphysics PDE systems. It is based on the decomposition of the computational domain (such as a nuclear reactor) into small geometrically simple objects (hexahedra, tetrahedra, prisms) called **finite elements**. In the finite elements the solution is approximated using polynomials with unknown coefficients. By inserting the polynomial approximation back into the original PDE, a system of linear or nonlinear algebraic equations is obtained. This system is typically very large (up to billions of equations). Computers used for FEM computations often have thousands of processors. Dr. Solin's group is known for their contributions in the area of **adaptive higher-order finite element methods** (***hp*-FEM**). The hp-FEM is capable of extremely fast, exponential convergence – often it is hundreds to thousand times faster than traditional FEM used in commercial programs.

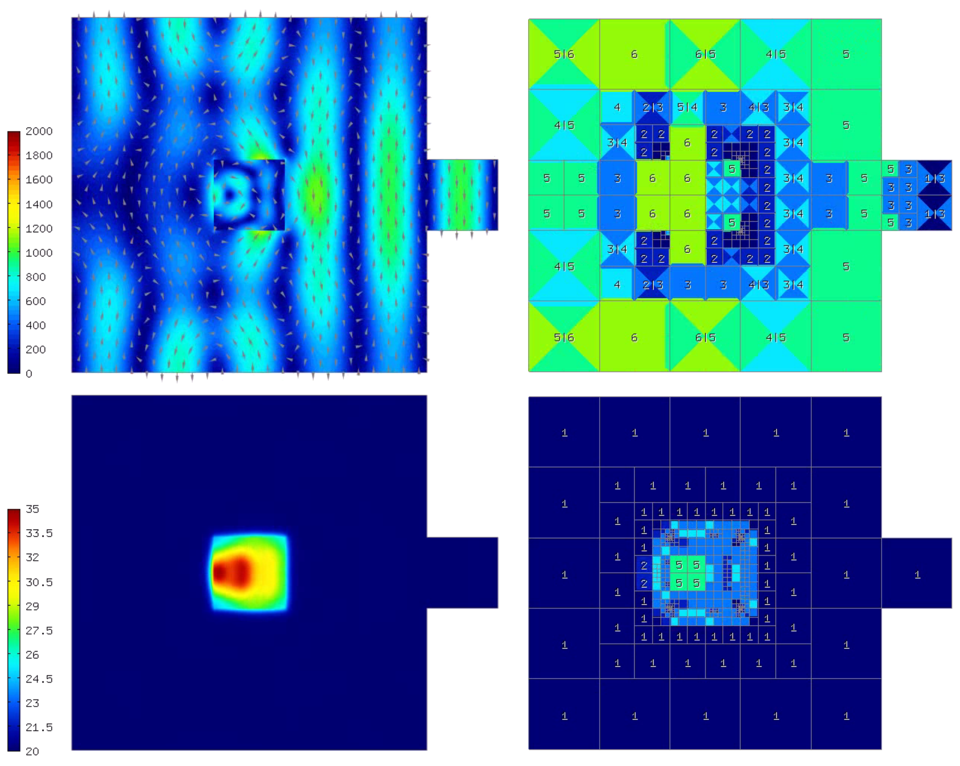
Novel Computational Techniques

Dr. Solin's group developed several unique computational techniques related to adaptive hp-FEM. These methods have been adopted by researchers at universities and national laboratories:

- **Arbitrary-level hanging nodes** enable rapid changes of scale in locally refined higher-order finite element meshes.
- **Multimesh *hp*-FEM** makes it possible to approximate various physical fields in multiphysics problems on individual meshes equipped with mutually independent adaptivity mechanisms.
- **PDE-independent adaptivity algorithms** based on general functional-analytic principles rather than on specific properties of PDE. This makes them easily applicable to arbitrary multiphysics PDE systems.
- **Adaptive *hp*-FEM with dynamical meshes** makes it possible to solve time-dependent problems efficiently and with controlled accuracy in both space and time.

Microwave Heating

In a microwave oven, electromagnetic waves are generated using time-harmonic current in a small cavity (on the right in the figure below). They enter a large cavity that contains an object with temperature-dependent material parameters. The electric field $\boldsymbol{E}$ deposits energy into the object, its temperature T rises, and this in turn changes the electric field. Mathematically, the process is modeled using the **Maxwell's equation** coupled with the **heat transfer equation**.



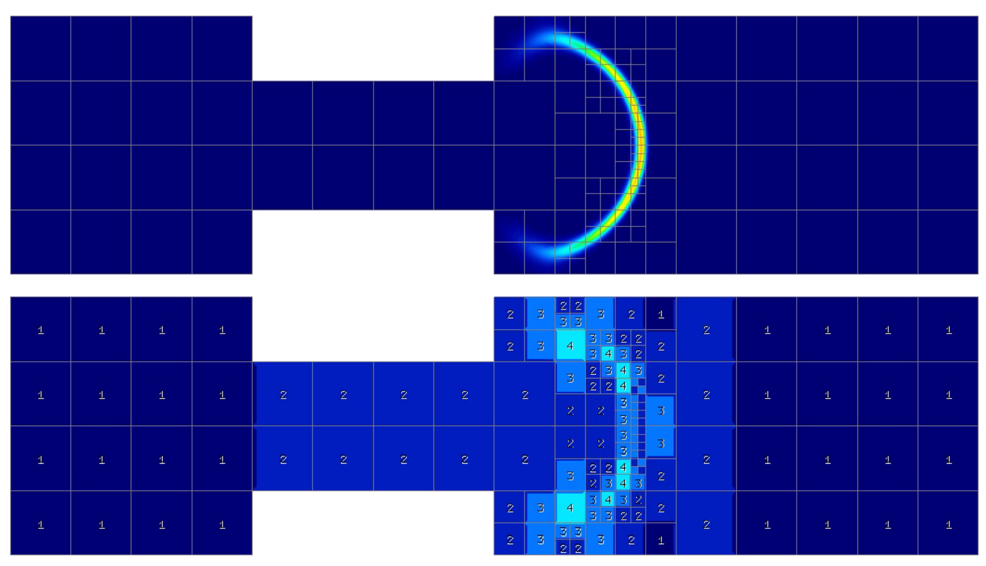
$\boldsymbol{E}$ and its mesh (top), T and its mesh (bottom).

Flame Propagation

Flame propagation problems are known to exhibit sharp fronts that travel through the computational domain (such as a burner) at high velocities. These problems pose extreme challenges to adaptive finite element methods. An example of such a problem (simplified) is a **pair of coupled nonlinear parabolic equations**

$$\frac{\partial T}{\partial t} - \Delta T = \omega(T,Y),$$
$$\frac{\partial Y}{\partial t} - \frac{1}{\mathrm{Le}}\Delta Y = -\omega(T,Y).$$

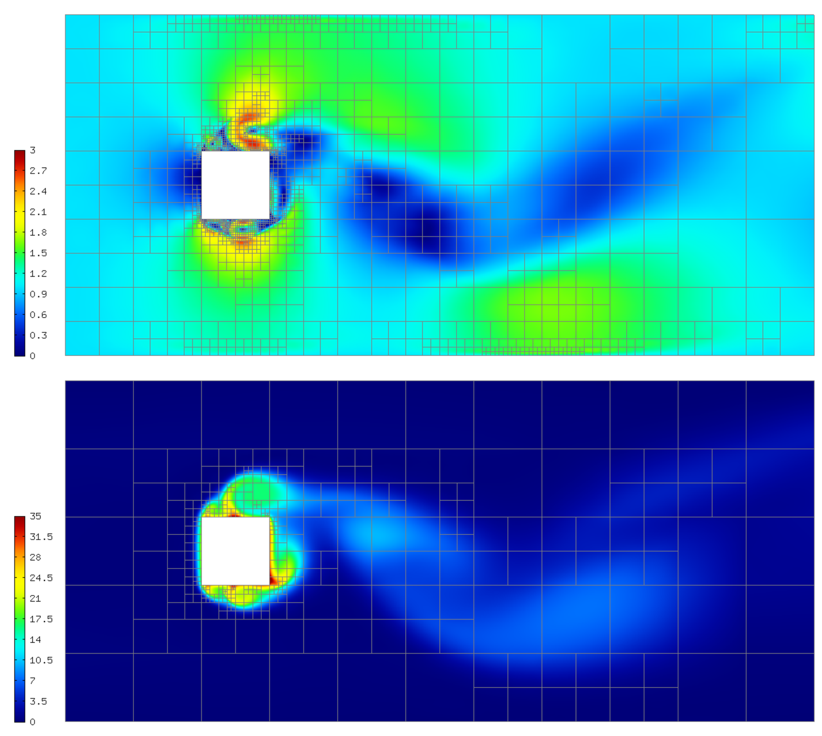
Here, T is the temperature, Y the concentration, Le the Lewis number. The reaction rate (flame intensity) ω is defined by the Arrhenius law.



Reaction rate ω and its mesh.

Reactor Coolant Flow

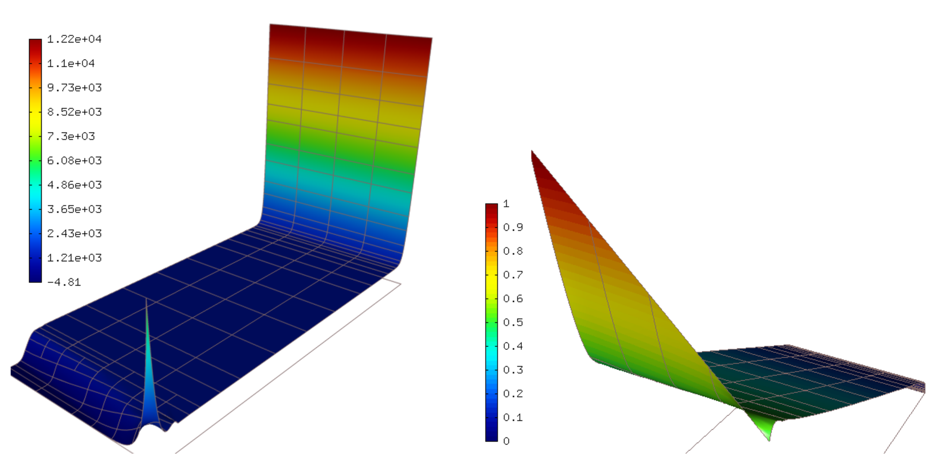
In nuclear reactors, kinetic energy of fission products is converted to thermal energy. A reactor coolant – usually water but sometimes a gas or a liquid metal or molten salt – is circulated past the reactor core to absorb the heat and generate steam. Depending on how the steam is generated, we distinguish between **boiling water reactors (BWR)** and **pressurized water reactors (PWR)**. The simulation shown below shows a coupled PDE system consisting of the **Navier-Stokes equations** and the **heat transfer equation**.



Coolant velocity $\boldsymbol{v}$ and temperature T.

Ionic Polymer-Metal Composites

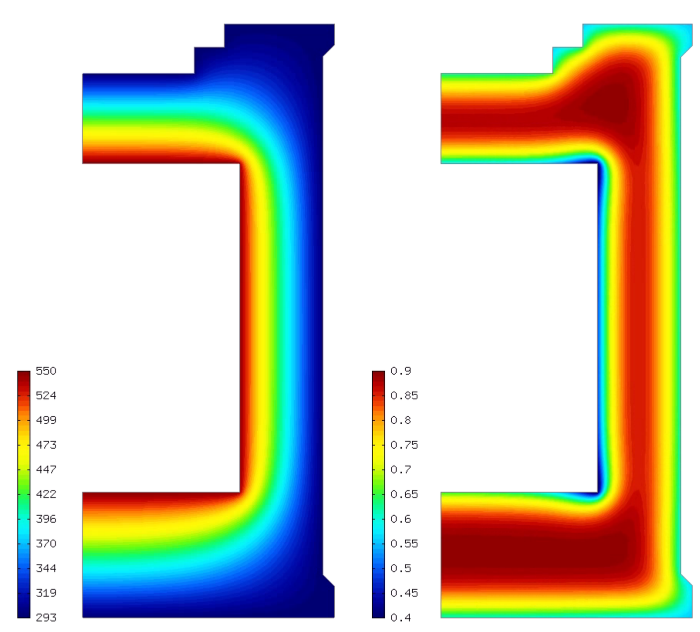
Ionic Polymer-Metal Composites (IMPC) are noiseless mechano-electrical and electro-mechanical transducers. The advantages of IPMC over other electroactive polymer actuators are low voltage bending, high strains (greater than 1%), and an ability to work in wet environments. A typical IPMC consists of a thin sheet of polymer (often Nafion or Teflon) which is sandwiched between noble metal electrodes such as platinum or gold. Mathematically, this is a coupled PDE system that includes the **Nernst-Planck equation** and the **Poisson equation**.



Positive ion concentration and voltage.

Hygro-Thermal Processes

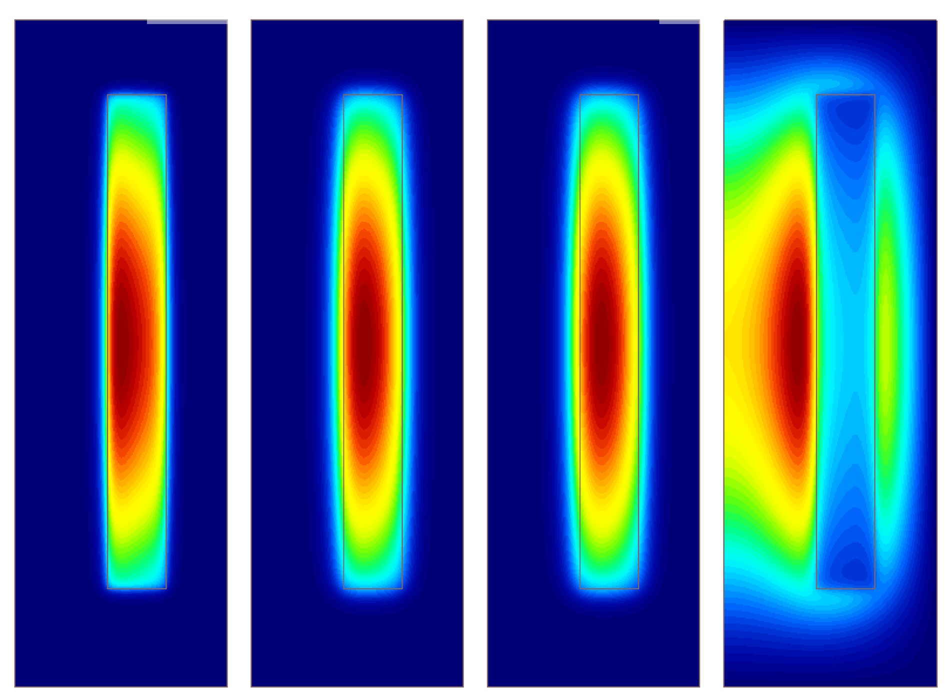
Massive concrete constructions such as nuclear reactor vessels undergo deformations and can crack when exposed to thermal loading (reactor heat). The figure below shows the distribution of temperature (left) and moisture (right) in a **nuclear reactor vessel** (axisymmetric 3D model). The height of the vessel is about 40 m and its walls are 5 – 7.5 m thick.



Temperature and moisture in a reactor vessel (axisymmetric model).

Multigroup Neutronics

Neutron flux in a reactor core comprises continuous spectrum of energies. In computations we restrict ourselves to several discrete **energy groups**. Mathematically, this is an **eigenproblem for the neutron diffusion equation**.



Sample solution of four-group neutronics.

Open Source Project HERMES

HERMES is a C++ library for rapid development of adaptive hp-FEM and hp-DG solvers. Novel hp-adaptivity algorithms are designed to solve a large variety of problems ranging from ODE and stationary linear PDE to complex time-dependent nonlinear multiphysics PDE systems. Detailed user documentation enhanced with many benchmarks and examples allow the users to employ HERMES without being experts in finite element methods or partial differential equations. Visit HERMES home page `http://hpfem.org/hermes`.

Acknowledgment

The research of Dr. Solin and his international group has been supported over the last ten years by the U.S. Department of Energy, U.S. Department of Defense, National Science Foundation, Sandia National Laboratory, Idaho National Laboratory, Lawrence Livermore National Laboratory, Grant Agency of the Czech Republic, and Grant Agency of the Academy of Sciences of the Czech Republic. The novel computational methods and results presented in this poster are the outcome of a joint effort of Dr. Solin, his research group, and external collaborators.

References

[1] L. Dubcova, P. Solin, J. Cerveny, P. Kus: Space and Time Adaptive Two-Mesh hp-FEM for Transient Microwave Heating Problems, Electromagnetics, Vol. 30, Issue 1, pp. 23 - 40, 2010.

[2] P. Solin, L. Dubcova, J. Kruis: Adaptive hp-FEM with Dynamical Meshes for Transient Heat and Moisture Transfer Problems, J. Comput. Appl. Math. 233 (2010) 3103-3112.

[3] P. Solin: *Partial Differential Equations and the Finite Element Method*, J. Wiley & Sons, Hoboken, 2005.