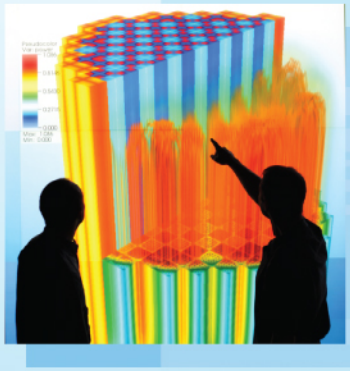
CASL-U-2014-0137-000

Power uprates
and plant life extension

Consortium for Advanced Simulation of LWRs



Engineering design
and analysis

Presentation Poster: A One-Dimensional Analysis of Anderson Acceleration for Coupled Neutronic and Thermal Hydraulic Calculations in a Light Water Reactor

Science-enabling
high performance
computing

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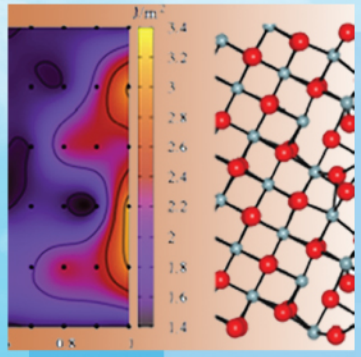
August 4, 2014



Fundamental science

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

A One-Dimensional Analysis of Anderson Acceleration for Coupled Neutronic and Thermal Hydraulic Calculations in a Light Water Reactor

Alex R. Toth – North Carolina State University

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Introduction

- Accurate simulation of light water reactors requires simultaneous solution of various coupled physical systems (e.g. neutronics, CFD, fuel properties).
- Couplings in CASL are generally implemented as Picard iterations.
- Picard iteration is implemented as a sequence of single-physics solves with the updated solution transferred to other sets of physics until convergence.
- Flexible implementation allows for use of existing codes in the VERA software package for accurate single physics solves.
- Interested in capturing the behavior of a Picard coupling between Insilico for Neutronics and AMP for fuel performance and subchannel flow.
- At high enough reactor power, oscillatory error modes arise in the solution, and numerical damping is required for convergent iteration. Would be ideal to utilize a more robust and faster converging solution method.
- Oscillatory behavior largely observed in axial direction, so we attempt to analyze convergence behavior with a 1D model which can be solved rapidly.

Model Description

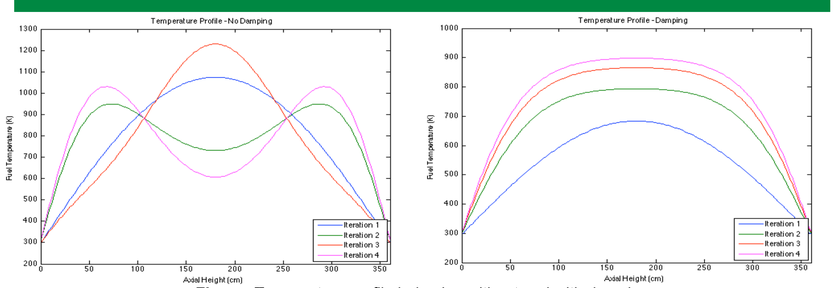

Figure: Temperature profile behavior, without and with damping

- Model coupling between neutronics and fuel and coolant properties in a single pin cell with height L, physical properties homogenous at each axial height.
- Neutron distribution governed by the diffusion equation:

$$-\frac{d}{dz}D\frac{d\phi}{dz} + (\Sigma_t - \Sigma_s)\phi(z) = \frac{1}{k}\nu\Sigma_f\phi$$

subject to the power normalization:

$$\frac{1}{L}\int_0^L E_f\Sigma_f\phi\,\mathrm{d}z = P^*$$

- Suppose axial conduction negligible in fuel, and fuel temperature governed by Newton's Law of Cooling:

$$2\pi Rh(T_f - T_w) = q'$$

where T_f is the fuel temperature and T_w is the coolant temperature.

- Consider both a two-way coupling between neutronics and fuel temperature, with constant coolant, and a three-way coupling integrating the flow model:

$$\dot{m}c_p\frac{\partial T_w}{\partial z} = q'$$

- We implement a Picard iteration as:

$$-\frac{d}{dz}D(T_f^n)\frac{d\phi^{n+1/2}}{dz} + (\Sigma_t(T_f^n) - \Sigma_s(T_f^n))\phi(z)^{n+1/2} = \frac{1}{k}\nu\Sigma_f(T_f^n)\phi^{n+1/2}$$

$$\phi^{n+1} = \frac{P^*\phi^{n+1/2}}{\frac{1}{L}\int_0^L E_f\Sigma_f(T_f^n)\phi^{n+1/2}\,\mathrm{d}z}$$

$$T_f^{n+1/2} = T_w + \frac{q'}{2\pi Rh}$$

$$T_f^{n+1} = (1-\omega)T_f^n + \omega T_f^{n+1/2}$$

- T_w is either taken to be constant or computed using the flow model, and ω is called the damping factor.
- Diffusion equation solved with Trilinos eigensolvers. Cell homogenized cross sections computed by linear fit from data points generated by XSProc.

Anderson Acceleration

- Acceleration method for solving the fixed point problem u = G(u).
- Stores at most m (user specified number) previous function evaluations and computes new iterate as the linear combination of these with minimal linearized residual:

$$u_{n+1} = (1-\beta)\sum_{j=0}^{m_n}\alpha_j^{(k)}u_{n-j} + \beta\sum_{j=0}^{m_n}\alpha_j^{(k)}G(u_{n-j})$$

where $m_n = \min\{m, n\}$, and $\{\alpha_j^{(n)}\}$ solves the constrained optimization problem

$$\min_{\{\alpha_j\}}\left\|\sum_{j=0}^{m_n}\alpha_j[G(u_{m-j}) - u_{m-j}]\right\|, \quad \text{subject to} \quad \sum_{j=0}^{n}\alpha_j = 1$$

- Call the algorithm with given m Anderson-m, β is called the mixing parameter.
- Same implementations requirements as Picard, only additional cost is storage of additional vectors.
- Anderson is "essentially equivalent" to GMRES iteration for linear problems.
- Anderson is locally linear convergent for nonlinear problems.
- We have implemented Anderson in the Trilinos nonlinear solver package NOX.

Two-Way Coupling Results

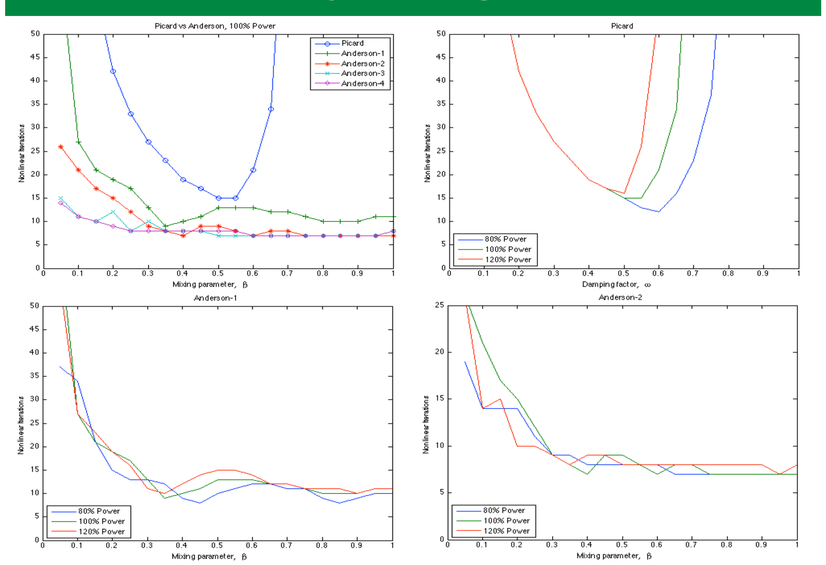

Figure: Picard and Anderson iterations to convergence, varying levels of damping

- The two-way Picard coupling displays the same oscillatory instabilities observed in the high-fidelity coupling. Without sufficient damping, the temperature and flux distributions alternate between single-peaked and double-peaked distributions.
- Oscillations in Picard iteration leads to slow convergence or divergence.
- The same oscillatory behavior is observed in the Anderson iterations, though it does not seem to adversely affect convergence.
- Iteration counts for Picard are similar to what has been observed in the Insilico/AMP coupling.
- The optimal level of damping for Picard is dependent on the power level. For reasonable power levels, an optimal choice is generally in the range 0.3-0.6.
- Anderson iterations are largely insensitive to the choice of mixing parameter. Convergence slowed if mixing parameter is too small, but range for what is optimal is much larger and ranges from about 0.3-1.0. This range appears to be insensitive to the power level.

Three-Way Coupling Results

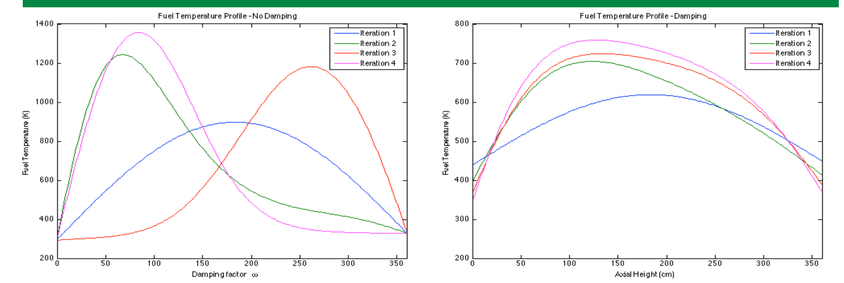

Figure: Fuel temperature profile behavior, without and with damping

- In implementation of the flow model, specific heat is interpolated from a table look-up.
- Without sufficient damping, oscillatory instabilities in Picard iteration now arise as a shift between front-peaked and back-peaked fuel temperature and flux. This results from asymmetry introduced into the problem by the flow model.
- Picard requires more damping, and optimal damping factor is about 0.3.
- Anderson-1 fails to converge for mixing parameters greater than 0.8.
- Other Anderson iterations are relatively insensitive to the mixing parameter, and there is no obvious trend for what would be an optimal value.

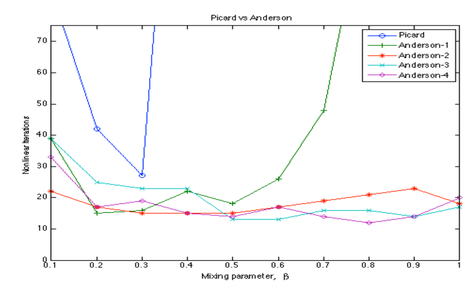

Figure: Picard and Anderson iterations to convergence, varying levels of damping

Conclusions and Future Work

- The simple model we have developed seems to capture the relevant axial instabilities observed in the Insilico/AMP coupling.
- Convergence behavior for the Picard iterations for both the high-fidelity coupling and this 1D model agree relatively well.
- Anderson is seen to be a faster converging, more robust method for this problem. Doesn't require a priori knowledge for selection of mixing parameter.
- Preliminary studies have been carried out implementing Anderson acceleration on the Insilico/AMP coupling.
  - At lower power, Anderson converges in approximately same number of iterations as optimally damped Picard.
  - At higher power, iterations fail due to violating bounds on material property evaluations.
  - In our model only specific heat calculation features this sort of bound, but coolant temperature never approaches violating the bounds.
  - It is then of interest to determine whether this failure mode would be observed with a better flow model, or if there is some way to address these bound failures (possibly implementing a line search on Anderson).

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