Accelerating Nonlinear PDE Solves through Residual-Based Enhancement of Surrogate Initial Guesses

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The numerical resolution of nonlinear partial differential equations (PDE) typically requires solving large-scale nonlinear algebraic systems of the form $\boldsymbol{F}(\boldsymbol{u}, \boldsymbol{\mu}) = \boldsymbol{0}$, where $\boldsymbol{u}$ denotes the solution vector and $\boldsymbol{\mu}$ denotes a vector of parameters.

To solve such problems, Newton and quasi-Newton methods, possibly combined with Krylov-subspace techniques (e.g., Generalized minimal residual (GMRES), Jacobian-Free Newton-Krylov (JFNK) schemes,...) remain standard tools for this task [1, 2].

Their efficiency, however, is highly sensitive to the quality of the initialization. In the absence of data, one typically uses a constant field that satisfies the boundary conditions. When previous resolutions across the same parameter space are available, a more effective strategy is to build a surrogate model from the resulting solutions. Methods from Non-Intrusive Reduced Order Models (NIROM) such as Proper Orthogonal Decomposition combined with Gaussian Process regression (POD-GP) are particularly well suited to this purpose [3].

Such a strategy accelerates the resolution by providing an initial guess that lies closer to the solution or near the quadratic convergence basin [4]. In many cases, this is still not sufficient, and the non-intrusive paradigm prevents any further improvement of the prediction itself.

We therefore shift the focus from directly predicting the initial guess to learning, in an offline stage, the corrective directions naturally produced along Newton trajectories. We propose a correction strategy that relies only on residual evaluations. The POD direction basis defines a Jacobian-free GMRES-type correction that refines the POD-GP initial guess at the cost of a handful of residual evaluations, before the result is handed over to the high-fidelity Newton solver, which then requires fewer expensive iterations. This residual-based step is no longer strictly non-intrusive, as it queries the full-order residual to inject problem-specific physics into the correction. Yet it remains far lighter than an intrusive POD–Galerkin approach, requiring only residual evaluations and no Jacobian.

Numerical experiments confirm the strong benefits of our approach.

A one-dimensional nonlinear elliptic boundary-value problem governed by the constitutive law $\varphi(\boldsymbol{s}) = -\kappa \boldsymbol{s} - \mu \boldsymbol{s}^5$ with $\kappa, \mu > 0$ is first considered. This model is then extended to the two-dimensional domain by applying the same constitutive law componentwise to the gradient:

$$\nabla \cdot (\boldsymbol{\varphi}(\nabla \boldsymbol{u})) = q_0, \qquad \boldsymbol{\varphi}(\nabla \boldsymbol{u}) = \left(\varphi(\partial_x \boldsymbol{u}), \varphi(\partial_y \boldsymbol{u})\right)^T,$$

subject to homogeneous Dirichlet boundary conditions. This componentwise extension yields a nonlinear orthotropic elliptic problem.

Numerical results indicate that the proposed POD-GMRES refinement reduces the number of full Newton iterations compared to the full Newton initialized by POD-GP only and reduces the overall CPU computation time.

Keywords: Generalized Minimal Residual (GMRES); Proper Orthogonal Decomposition (POD); Quasi-Newton methods; Non-intrusive reduced-order modeling; Solver initialization

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