Spectral Element Multigrid

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Multigrid Concepts

- Physics-based preconditioning is used to reduce the order of matrices and make them elliptic and diagonally dominant.
- Multigrid provides a scalable parallel method for solving diagonally-dominant matrices.
- Coarsening and refining strategies
  - Classical grid-based methods (CMG): coarser and finer grids.
    Not suitable for spectral elements.
  - Algebraic multigrid (AMG): choose largest matrix elements for coarsening.
    PETSc/Hypre/BoomerAMG. Tested for spectral elements, unsuccessful.
  - Spectral element multigrid (SEMG): specifically designed for spectral elements,
    uses higher and lower polynomial degrees within each grid cell.
- Smoothers
  - Krylov smoother is used to verify multigrid framework. Effective but not scalable.
  - Jacobi smoother. Diagonal dominance is a property of the nodal basis. Coarsening and refining is easiest in the modal basis. We work back and forth between them.
  - SuperLU is used on the coarsest level. Could use other PETSc solvers, e.g. classical multigrid.
- References
  - E. M. Ronquist and A. T. Patera, "Spectral Element Multigrid I: Formulation and Numerical Results," J. Sci. Comput. **2**, 4, 389-406 (1987).
  - Y. Madera and R. Munoz, "Spectral Element Multigrid II: Theoretical Justification," J. Sci. Comput. **3**, 4, 323-353 (1988).

Abstract Multigrid Algorithm

Abstract Elliptic Problem

Hilbert space $\mathcal{H}$, bilinear elliptic form a, linear form g.

$$\text{Find } v \in \mathcal{H} \text{ such that } \quad \forall u \in \mathcal{H}, \quad a(u,v) = g(u)$$

Nested Finite-Dimensional Subspaces

$$\mathcal{M}_1 \subset \mathcal{M}_2 \subset \cdots \subset \mathcal{M}_j \subset \mathcal{H} \quad \text{Simplest case } j = 1, 2.$$

$$\text{Find } v_j \in \mathcal{M}_j \text{ such that } \quad \forall u \in \mathcal{M}_j, \quad a(u, v_j) = g(u)$$

Smoother

$b(u,v) \approx a(u,v)$, but easier to solve, *e.g.* Jacobi smoother, $b \sim \mathrm{Diag}(a)$.

Multigrid V-Cycle

1. $m/2$ smoother iterations. Find $\mathcal{S}\varphi \in \mathcal{M}_2$ such that
$$\forall u \in \mathcal{M}_2, \quad a(u, \mathcal{S}\varphi - \varphi) = g(u) - a(u, \varphi)$$
2. Coarse correction. Find $\bar{\varphi} \in \mathcal{M}_1$ such that
$$\forall u \in \mathcal{M}_1, \quad a(u, \mathcal{S}\varphi - \bar{\varphi}) = g(u) - a(u, \varphi), \quad \mathcal{C}\varphi \equiv \varphi + \bar{\varphi}$$
3. $m/2$ smoother iterations.

Operator Expression

$$u^1 = \mathcal{S}^{m/2} \mathcal{C} \mathcal{S}^{m/2} u^0$$

Convergence Theorem

Generalized Eigenvalue Problem

$$\forall u \in \mathcal{M}_1, \quad a(u, \Psi_i) = \lambda_i b(u, \Psi_i)$$

$$\text{Rescale } b \rightarrow \frac{b}{\lambda_{\max}}, \quad 0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_P = 1$$

Nesting Hypothesis

The fine space is the span of all P eigenvectors, $\mathcal{M}_2 = \{\Psi_1, \Psi_2, \ldots, \Psi_P\}$.

The coarse space is the span of the lowest p eigenvectors, $\mathcal{M}_1 = \{\Psi_1, \Psi_2, \ldots, \Psi_p\}$.

Convergence Theorem

Let $e^j \equiv u - u^j$, the error after the jth iteration.

$$a(e^1, e^1) \leq (1 - \lambda_{p+1})^{2m} a(e^0, e^0)$$

Interpretation

The largest "rough" eigenvalues, closest to 1, converge rapidly.

The smallest "smooth" eigenvalues, closest to 0, converge slowly.

The coarse correction eliminates the smooth eigenvalues
by transferring them to a coarse grid and solving exactly.

Analytical Test Case

1D Poisson Equation

$$-u''(x) = g(x), \quad u(x) = 0 \text{ at } x = \pm 1$$

Convergence Theorem

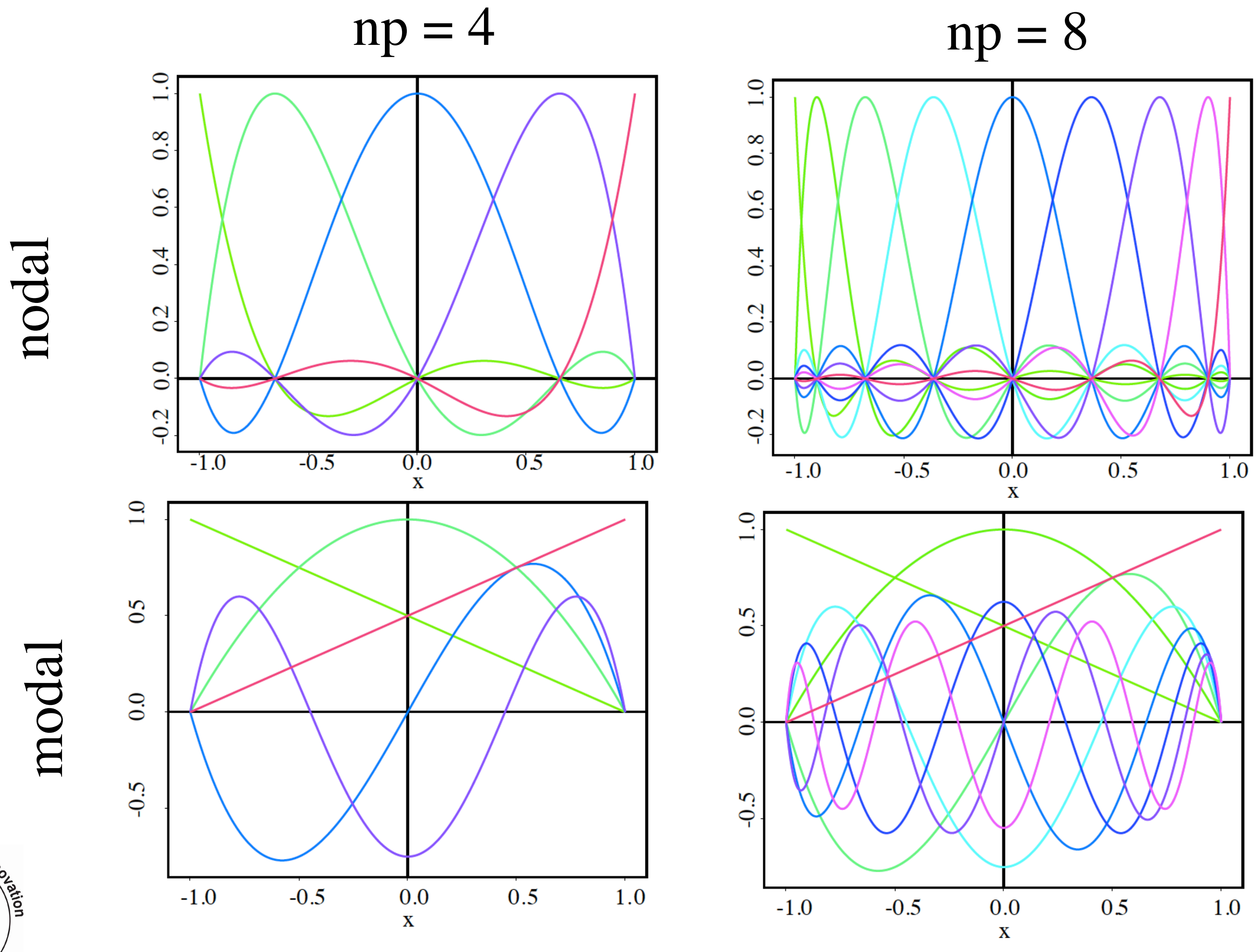
Using the Lobatto nodal basis functions of degree N,
with the scaled diagonal matrix as the smoother,
convergence for one element and 2 levels is given by

$$a(u - u^1, u - u^1) = \mu a(u - u^0, u - u^0)$$

$$\mu = \left[1 - \frac{N+2}{2(N-1)}\right]^{2m}$$

$$\mu < 1 \text{ for } N > 2$$

Nodal and Modal Bases: Pictures



Nodal and Modal Bases: Equations

Lobatto Nodal Basis Functions

$$u(x) = u_i \alpha_i(x), \quad x \in (-1,1), \quad i = 0, \ldots, n$$

$$\alpha_i(x) \equiv \prod_{j \neq i} \left(\frac{x - x_j}{x_i - x_j} \right), \quad (1 - x_i^2) P_n^{(0,0)\prime}(x_i) = 0$$

Jacobi Modal Basis Functions

$$u(x) = \bar{u}_j \beta_j(x), \quad x \in (-1,1), \quad j = 0, \ldots, n$$

$$\beta_0(x) \equiv \frac{1-x}{2}, \quad \beta_n(x) \equiv \frac{1+x}{2}$$

$$\beta_j(x) \equiv (1 - x^2) P_{j-1}^{(1,1)}(x), \quad j = 1, \ldots, n-1$$

Change of Basis

$$u_i = u(x_i) = \bar{u}_j \beta_j(x_i) = T_{ij} \bar{u}_j, \quad T_{ij} \equiv \beta_j(x_i)$$

Matrix-Vector Form

$$\mathbf{u} \equiv \{u_i\}, \quad \bar{\mathbf{u}} \equiv \{\bar{u}_j\}, \quad \mathbf{T} \equiv \{T_{ij}\}, \quad \mathbf{u} = \mathbf{T}\bar{\mathbf{u}}, \quad \bar{\mathbf{u}} = \mathbf{T}^{-1}\mathbf{u}$$

Coarsening and Refining

Coarsen and Refine, Modal Bases

$$u^m(x) = \sum_{i=0}^{m} \bar{u}_i^m \beta_i^m(x), \quad u^n(x) = \sum_{i=0}^{n} \bar{u}_i^n \beta_i^n(x), \quad m < n$$

$$\bar{u}_i^m = \bar{u}_i^n, \quad i = 0, \dots, m-1; \quad \bar{u}_m^m = \bar{u}_n^n$$

$$\bar{u}_i^m = \bar{C}_{ij}^{mn} \bar{u}_j^n, \quad i = 0, \dots, m, \quad j = 0, \dots, n$$

$$\begin{aligned} \bar{C}_{ij}^{mn} &= \delta_{ij}, \ j = 0, \dots, m-1 \\ &= 0, \ j = m, \dots, n-1 \\ &= \delta_{im}, \ j = n \end{aligned}$$

$$\bar{\mathbf{C}}^{mn} = \{\bar{C}_{ij}^{mn}\}, \quad \bar{\mathbf{u}}^m = \bar{\mathbf{C}}^{mn} \bar{\mathbf{u}}^n$$

$$\bar{\mathbf{R}}^{nm} = (\bar{\mathbf{C}}^{mn})^T, \quad \bar{\mathbf{u}}^n = \bar{\mathbf{R}}^{nm} \bar{\mathbf{u}}^n$$

Coarsen and Refine, Nodal Bases

$$\mathbf{u}^m = \mathbf{T}^m \bar{\mathbf{u}}^m = \mathbf{T}^m \bar{\mathbf{C}}^{mn} \bar{\mathbf{u}}^n = \mathbf{T}^m \bar{\mathbf{C}}^{mn} (\mathbf{T}^n)^{-1} \mathbf{u}^n = \mathbf{C}^{mn} \mathbf{u}^n$$

$$\mathbf{u}^n = \mathbf{T}^n \bar{\mathbf{u}}^n = \mathbf{T}^n \bar{\mathbf{R}}^{nm} \bar{\mathbf{u}}^m = \mathbf{T}^n \bar{\mathbf{R}}^{nm} (\mathbf{T}^m)^{-1} \mathbf{u}^m = \mathbf{R}^{nm} \mathbf{u}^m$$

$$\mathbf{C}^{mn} = \mathbf{T}^m \bar{\mathbf{C}}^{mn} (\mathbf{T}^n)^{-1}, \quad \mathbf{R}^{nm} = \mathbf{T}^n \bar{\mathbf{R}}^{nm} (\mathbf{T}^m)^{-1} \neq (\mathbf{C}^{mn})^T$$

Test Case: Poisson's Equation, Stiffness Matrix

Nodal and Modal Representations

$$(u, Lv) \equiv -\int_{-1}^{1} dx\, u \frac{\partial^2 v}{\partial x^2} = \int_{-1}^{1} dx \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} = u_i L_{ij} v_j = \bar{u}_k \bar{L}_{kl} \bar{v}_l$$

$$L_{ij} \equiv \int_{-1}^{1} dx \frac{\partial \alpha_i}{\partial x}\frac{\partial \alpha_j}{\partial x}, \quad \bar{L}_{ij} \equiv \int_{-1}^{1} dx \frac{\partial \beta_i}{\partial x}\frac{\partial \beta_j}{\partial x}$$

$$u_i L_{ij} v_j = (T_{ik}\bar{u}_k) L_{ij} (T_{jl}\bar{v}_l) = \bar{u}_k (T_{ik} L_{ij} T_{jl}) \bar{v}_l = \bar{u}_k \bar{L}_{kl} \bar{v}_l$$

$$\bar{L}_{kl} = T_{ik} L_{ij} T_{jl}, \quad \bar{\mathbf{L}} = \mathbf{T}^{\dagger}\mathbf{L}\mathbf{T}, \quad \mathbf{L} = \mathbf{T}^{\dagger -1}\bar{\mathbf{L}}\mathbf{T}^{-1}$$

Nodal and Modal Coarsening

$$(u, Lv)^m \equiv -\int_{-1}^{1} dx\, u^m \frac{\partial^2 v^m}{\partial x^2} = \int_{-1}^{1} dx \frac{\partial u^m}{\partial x}\frac{\partial v^m}{\partial x} = u_i^m L_{ij}^m v_j^m$$

$$(u, Lv)^n \equiv -\int_{-1}^{1} dx\, u^n \frac{\partial^2 v^n}{\partial x^2} = \int_{-1}^{1} dx \frac{\partial u^n}{\partial x}\frac{\partial v^n}{\partial x} = u_k^n L_{kl}^n v_l^n$$

$$L_{ij}^m \equiv \int_{-1}^{1} dx \frac{\partial \alpha_i^m}{\partial x}\frac{\partial \alpha_j^m}{\partial x}, \quad i, j = 1, \ldots, m$$

$$L_{kl}^n \equiv \int_{-1}^{1} dx \frac{\partial \alpha_k^n}{\partial x}\frac{\partial \alpha_l^n}{\partial x}, \quad k, l = 1, \ldots, n$$

$$u_i^m L_{ij}^m v_j^m = R_{ki}^{nm} u_i^m L_{kl}^n R_{lj}^{nm} v_j^m$$

$$L_{ij}^m = R_{ki}^{nm} L_{kl}^n R_{lj}^{nm}, \quad \mathbf{L}^m = (\mathbf{R}^{nm})^T \mathbf{L}^n \mathbf{R}^{nm}$$

Implementation and Status

- Spectral element multigrid is implemented in Fortran 95 module `p2_semg.F`, using PETSc for distributed parallel operation and high-level matrix operations.
- Fortran 95 derived types are defined for multigrid levels, diagonal blocks matrices, scatter contexts between native and PETSc vectors, and a full SEMG problem.
- Subroutine p2_semg_transform is used to transform between modal and nodal bases and for coarsening and refining, using low-order (np+1) matrices $\mathbf{T}$, $\mathbf{T}^{-1}$, $\mathbf{R}$, and $\mathbf{C}$.
- A multigrid sawtooth cycle is performed iteratively, with a full SuperLU direct solve on the coarsest level and a Krylov or Jacobi smoother on each of the finer levels.
- The formulation is general. Current test problem is 1D Poisson equation. Following this, it will be tested on:
    - 2D Poisson equation.
    - Simple linear 2D wave equation.
    - Ideal MHD waves in a periodic plane.
    - GEM challenge problem, magnetic reconnection.
    - 3D implementation and testing.
- Multigrid operation has been successfully tested with Krylov smoother.
- Jacobi smoother has been set up and tested, not yet fully debugged.
  Boundary condition problem
- Hope to complete 2D implementation and testing by APS/DPP.