Algorithms of Scientific Computing

Hierarchical Methods and Sparse Grids

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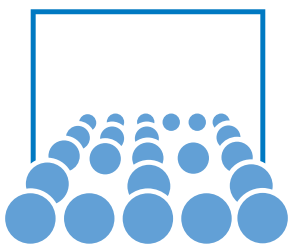


Part IX

Multigrid Methods

Multigrid Methods

Up to now we have considered

- Hierarchical bases (and algorithms) to represent functions with low costs as well as possible for
  - interpolation and quadrature,
  - the solution of a system of linear equations stemming from a PDE discretization

We haven't considered so far

- The solution of the system of linear equations
- There, hierarchical methods play a very important role
- Especially *multigrid methods* allow efficient iterative methods to solve linear system for important classes of discretized problems
- We will now consider multigrid (MG) methods
- But before, we have to look at classical iteration methods (esp. at their rates of convergence) to be able to evaluate multigrids

System of Linear Equations

- Aim: solve linear system

$$Ax = b \text{ with } A \in \mathbb{R}^{n \times n} \text{ and } x, b \in \mathbb{R}^n$$

- We assume that n is so large that a direct solution (with Gaussian elimination, e.g.) is too expensive regarding time or space
- As usual, we assume that A is sufficiently well-behaved
  - Typically desired properties: invertible, symmetric, with non-zero entries on diagonal, ...

Iterative Solvers

- Iterative solvers compute sequence of approximations

$$x^0, x^1, x^2, \ldots$$

- Converges against solution x of $Ax = b$
- In practice: stop method after finite number of steps; take iterate as approximation of x
- An iterative method will make compromise as well as possible between two requirements
  - x^{i+1} should be cheap to be computed out of $x^0, \ldots, x^i$ $\Rightarrow$ in the majority of cases: x^{i+1} is function only of x^i (and, of course, of A and b) – just consider storage space
  - Convergence should be as fast as possible: accurate results after as few steps as possible

Residual and Error

- For further considerations, the following notions are helpful:
  - The *residual* after i steps is defined as $r^i := b - Ax^i$
  - The *error* is $e^i := x^i - x$
- Residual easy to compute, but we would like to know error (would directly provide access to exact solution)
- Both magnitudes are related via equation $r^i = -Ae^i$
- This suggests to compute estimate of error out of residual:
  - Apply (cheap) approximation of $-A^{-1}$ on residual

  (Outlook for hierarchical methods: approximation can be obtained cheaply on coarser grid)

Linear Iterative Methods

Linear method to solve linear systems

- Can be written as

$$x^{i+1} = Mx^i + Nb \tag{1}$$

- M and N are $n \times n$ matrices
- M and N depend only on A, not on b or x^i
- Linear iterative methods are popular for several reasons (their analysis is relatively easy, e.g.)

Linear Iterative Methods: Consistency

Minimal requirement at iterative method:

- Exact solution has to be fixed point of iteration
- If we provide solution as x^0 it should not be destroyed
- Thus, for all b and a with $Ax = b$ it has to hold

$$x \stackrel{!}{=} Mx + Nb = (M + NA)x$$

$$\Rightarrow$$

$$M + NA = I \tag{2}$$

(as we can choose b and thus x arbitrarily)

- This requirement is called *consistency*

Linear Iterative Methods: Convergence

- With the consistency requirement $M + NA = I$ (2), we rewrite the iteration scheme $x^{i+1} = Mx^i + Nb$ (1) as

$$\begin{aligned} x^{i+1} &= (I - NA)x^i + Nb \\ &= x^i - N(Ax^i - b) \\ &= x^i + Nr^i \end{aligned}$$

- For the error, this results to

$$\begin{aligned} e^{i+1} = x^{i+1} - x &= x^i - x + Nr^i \\ &= e^i - NAe^i = Me^i \end{aligned}$$

Linear Iterative Methods: Convergence (2)

- Therefore, speed of convergence of iteration depends on M, more accurately on the norm of M:

$$\|e^{i+1}\| \leq \|M\| \cdot \|e^i\|$$

$\Rightarrow$ $\|M\|$ should be smaller than 1; the closer to 0 the better

First try

- We therefore choose $M := 0$
- The iterative method solves the linear system in the first step:

$$x^1 = x$$

- As expected, there is no free lunch, as

$$N = (I - M)A^{-1} = A^{-1}$$

- We would have to solve our linear system to compute $x^1 \ldots$

Jacobi Method

- We obtain feasible methods by the decomposition

$$A =: D - E - F$$

  where
  - D contains the diagonal of A,
  - $-E$ the (strictly) lower triangular part, and
  - $-F$ the (strictly) upper triangular part
- As an example, we look at the *Jacobi method*

A short remark:

- For sparse grids, we have mentioned the conjugated gradient method (CG)
- It is not a linear iterative method, but behaves rather similar

Jacobi Method (2)

- The Jacobi method chooses

$$N := D^{-1},$$

thus

$$M = I - D^{-1}A$$

- This results in the following algorithm:

  Compute x^{i+1} out of x^i:

  Compute residual $r^i := b - Ax^i$

  for $k = 1, \ldots, n$:

  $$x_k^{i+1} = x_k^i + \frac{1}{a_{k,k}} r_k^i$$

  endfor

- Computing r^i is, of course, a loop over all components, too
- But the matrix could be as well provided as a procedure allowing to compute matrix-vector products $x \mapsto Ax$
- Additionally, we only need knowledge about diagonal entries $a_{k,k}$

Jacobi Method (3)

- Unfortunately, we do not have convergence for arbitrary A
- In practice, one often introduces a damping factor $0 < \alpha \leq 1$ for the modification $D^{-1} r^i$ to obtain convergence
- If α is too small this goes at the expense of speed
- In the algorithm this looks like

$$\begin{aligned} &\dots \\ &x_k^{i+1} = x_k^i + \alpha \frac{1}{a_{k,k}} r_k^i \\ &\dots \end{aligned}$$

- For the matrices we obtain

$$N(\alpha) = \alpha D^{-1}$$

and

$$M(\alpha) = I - \alpha D^{-1} A$$

Speed of Convergence

How many iterations do we need to perform to obtain sufficiently small convergence error?

- We can obtain propositions about speed of convergence from equation

$$e^{i+1} = Me^i$$

- To simplify things we assume
  - M has a full set of eigen vectors $\eta_1, \ldots, \eta_n$ for real-valued eigen values $\lambda_1, \ldots, \lambda_n$
  - In reality, this does not always hold; but the concepts from the simplified case remain mainly the same

Speed of Convergence (2)

- We then can write e^0 as linear combination of eigen vectors

$$e^0 := \sum_{k=1}^{n} \beta_k \eta_k.$$

- Iterating (applying M) multiplies each component with corresponding λ_i

$$e^i = \sum_{k=1}^{n} \lambda_k^i \beta_k \eta_k.$$

- Typically, some of the eigen values are close to 0
  - $\Rightarrow$ The corresponding components decay very fast: at first, convergence makes a lot of progress

Speed of Convergence (3)

- Unfortunately, there are eigen values with absolute value just slightly below 1
  - The corresponding components of the error are hardly reduced
  - They dominate after few iterations the whole progress which becomes very slow after the first progress
- This effect is widely independent of x^0:
  - Error contains almost always components of all eigen vectors
  - If not: introduced at the latest by rounding errors

Speed of Convergence (4)

- Be λ_n the eigen value with absolute value closest to 1, thus

$$\delta := 1 - |\lambda_n|$$

  (unfortunately) close to 0
- Then it is for sufficiently many iterations

$$\frac{\|e^{i+1}\|}{\|e^i\|} \approx 1 - \delta.$$

- Number of iterations to obtain

$$\|e^{i+n_{it}}\| < \epsilon \|e^i\|$$

  for given $0 < \epsilon < 1$:

$$n_{it} \approx \frac{\ln \epsilon}{\ln(1-\delta)} \approx \frac{-\ln \epsilon}{\delta}$$

  (Expansion at $\delta = 0$ leads to $\ln(1-\delta) \doteq -\delta$)

Speed of Convergence (5)

- Unfortunately, we obtain for the discretization of PDEs on a grid with mesh-width h typically $\delta \sim h^{\gamma}$ for some $\gamma > 0$

$\Rightarrow$ The number of steps grows with $h^{-\gamma}$

- Even if the cost per step is proportional to number of unknowns, the overall effort grows disproportionally high

Speed of Convergence, Example

Example: damped Jacobi

- We solve linear system for discretized one-dimensional Poisson equation
  - Poisson equation $-u'' = f$
  - Stencil $\frac{1}{h^2}[-1\ 2\ -1]$

  on grid with $m-1$ inner grid points (zero on boundary)
- We solve linear system with damped Jacobi

$$x^{i+1} := x^i + \alpha D^{-1} r^i \quad \text{and} \quad 0 < \alpha \leq 1$$

Speed of Convergence, Example (2)

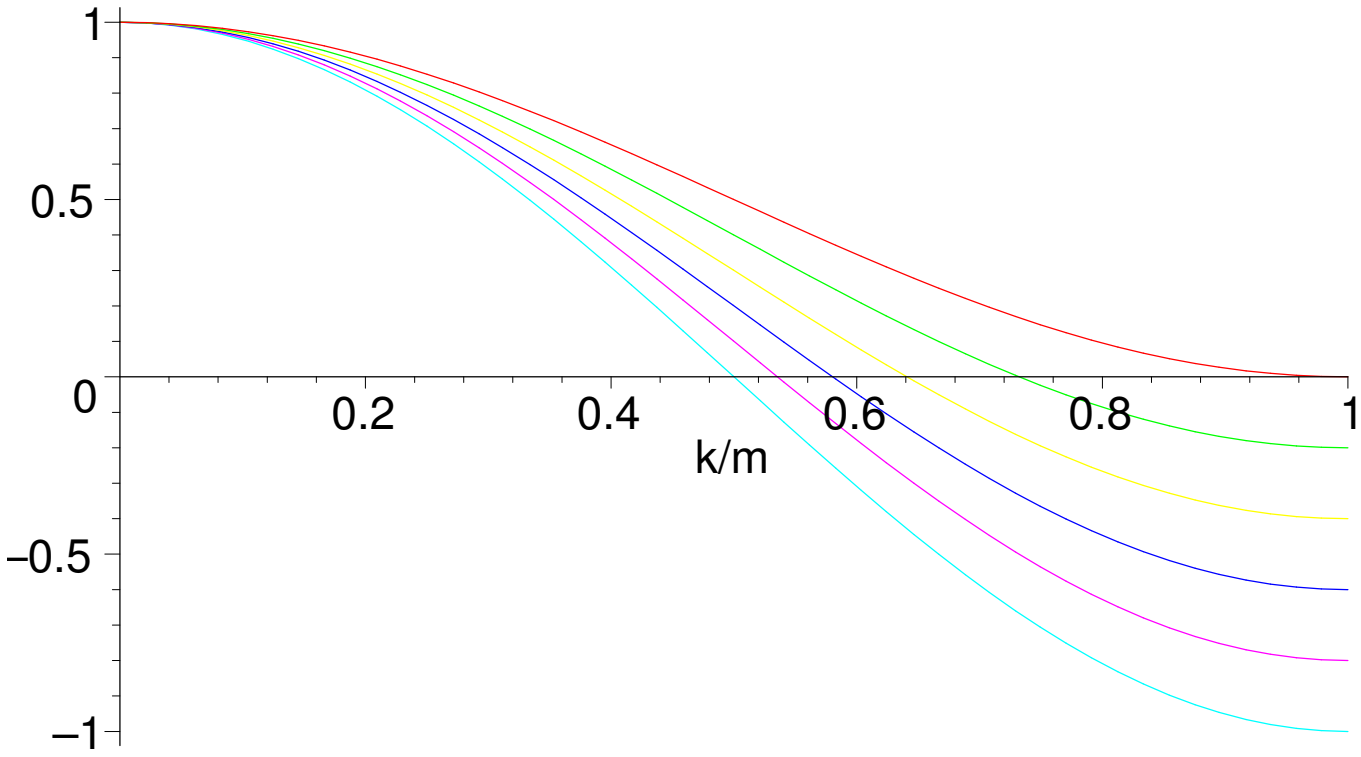
- The iteration matrix $M^{Jac} := I - \alpha D^{-1} A$ has as eigen vectors the discrete sine oscillations

$$\eta^k := \left(\sin\left(\frac{ik\pi}{m} \right) \right)_{1 \leq i < m} \in \mathbb{R}^{m-1}$$

- The corresponding eigen values are

$$\lambda_k := \alpha \cos\left(\frac{k\pi}{m} \right) + 1 - \alpha = 1 - 2\alpha \sin^2\left(\frac{k\pi}{2m} \right)$$

Speed of Convergence, Example (3)



Eigen values of M^{jac} for different values of $\alpha \in [0.5, 1]$

Speed of Convergence, Example (4)

- In the diagram, we can observe eigen values for low-frequency error components (k/m small)
- They are practically independent of α and very close to 1
- Closest to one is

$$\lambda_1 := 1 - 2\alpha \sin^2\left(\frac{\pi}{2m}\right) \doteq 1 - \frac{\alpha\pi^2}{2m^2}.$$

- At the right end of the diagram: eigen values to high-frequency error components ($k/m \approx 1$)
- We can adjust damping via α
  - $\alpha > 0.5$ results in oscillations (negative eigen values)
  - Convergence deteriorates with $\alpha \to 1$
- For all $0 < \alpha \leq 1$, the convergence rate is determined by λ_1

$\Rightarrow$ $\delta \in \mathcal{O}(m^{-2})$: half the mesh-width results in four times as many iterations for given error reduction

Why is Jacobi so Slow?

Summarizing the main observations

- For α suitably chosen, we can damp high-frequency error components ($k/m \to 1$) very well
- For all values of α, the low-frequency error components remain almost undamped

- We could have assumed that as low-frequency error terms produce only very small residuals
- Thus, residuum is not a very well-suited measure to construct estimate of error
- Remark: Related methods, such as Gauss-Seidel, therefore behave similarly

Why is Jacobi so Slow? (2)

- Further search for reasons of this problem lead to observation
  - Different error components (frequencies) have completely different relations between error e^i and residual $r^i = -Ae^i$
- This can be expressed as
  - A has a large condition number

$$\kappa(A) = \frac{\max\limits_{\|x\|=1} \|Ax\|}{\min\limits_{\|x\|=1} \|Ax\|}$$

(not so large that we get problems with accuracy of solution, but large enough to make iterative solution annoyingly slow)

Why is Jacobi so Slow? (3)

- Where does large condition number come from?
  - Not a property of our problem (solve a DE), but of discretization!
- For same problem, discretizations can be provided leading to arbitrary well-conditioned coefficient matrices
- Taking hierarchical basis (for a suitable scaling) leads to matrices with significantly better condition

- In the following, we proceed otherwise
- We kind of try to remedy the gaucheness during discretization with as little computational effort as possible
- The original problem with its properties will play an important role:
  - (Geometric) multigrid methods as treated here cannot be considered independent of problem

Multiple Grids

- A_h: coefficient matrix of example problem for mesh width $h = 1/m$
- Condition number of A_h is in $\mathcal{O}(h^{-2}) \Rightarrow$ gets worse with $h \to 0$
- But need small h to keep discretization error low

$\Rightarrow$ Take solutions of coarser grids for solution on current grid

- We will have to deal with family of linear systems on interval $[0, 1]$:

$$A_h x_h = b_h$$

for mesh-width $h = 2^{-l}$ as index for discretization level $l = l_{\min}, \ldots, l_{\max}$

Multiple Grids (2)

- Solutions on different grids represented by vectors of different length
- To be able to compare them, we decompose h-grid into
  - *coarse grid points*, which also exist on $2h$-grid
  - *fine grid points*, which don't
- The *prolongation* operator

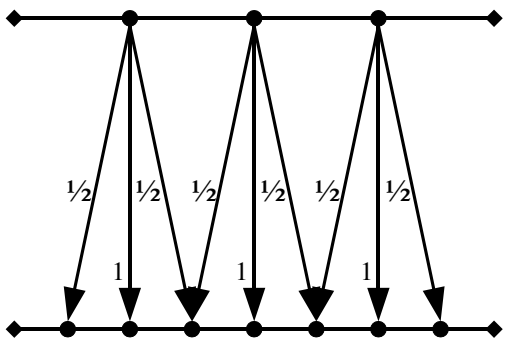
$$I_{2h}^{h} : \mathbb{R}^{1/(2h)-1} \rightarrow \mathbb{R}^{1/h-1},$$

  maps a u_{2h} on a $2h$-grid to a u_h on the h-grid
- The u_h
  - takes the values of u_{2h} at the coarse grid points and
  - interpolates the values at fine grid points linear out of coarse grid points (or boundary values, resp.)

Prolongation Operator

- As matrix and picture it looks as follows

$$I_{2h}^{h} = \frac{1}{2} \begin{pmatrix} 1 & & & \\ 2 & & & \\ 1 & 1 & & \\ & 2 & \ddots & \\ & 1 & \ddots & 1 \\ & & \ddots & 2 \\ & & & 1 \end{pmatrix}$$



Multiple Grids (cont.)

- Compare x_h with $I_{2h}^h x_{2h}$:
  - The difference will be small and mainly high-frequency
  - The low-frequency parts of the exact solution can be represented well on $2h$-grid
- Therefore straightforward to use $I_{2h}^h x_{2h}$ as initial solution for iteration on h-grid, so that contributions of resistant error modes small:

  Solve for $h = 2^{-l_{min}}$ linear system $A_h x_h = b_h$.
  for $l = l_{min} + 1, \ldots, l_{max}$:
  Iterate with $h = 2^{-l}$ and $x_h^0 := I_{2h}^h x_{2h}$
  the linear system $A_h x_h = b_h$ sufficiently often,
  call the result (afflicted with remaining error) x_h
  endfor

Multigrids

- Idea goes in right direction, but not far enough for most problems:
  - $I_{2h}^{h} x_{2h}$ contains – even if $A_{2h} x_{2h} = b_{2h}$ solved exactly – low-frequency error components, too

  $\Rightarrow$ Still many iterations on fine grid necessary if very accurate solution desired
- Thus, modify scheme so that coarse grids can be used multiple times to compute suitable correction
- Main idea:
  - After some iterations on fine grid, solve auxiliary equation which combines error and residual,

$$r^i = -Ae^i \,,$$

approximately for e^i on coarse grid

Multigrids (2)

- We need another operator, the *restriction*

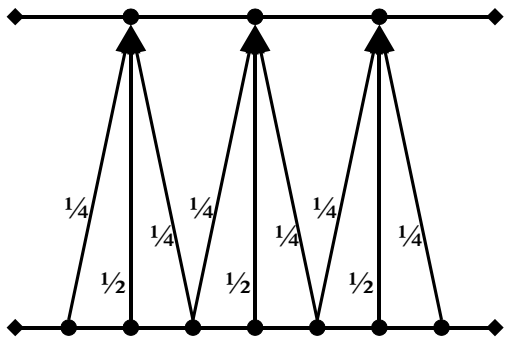
$$R_h^{2h} : \mathbb{R}^{1/h-1} \to \mathbb{R}^{1/(2h)-1},$$

- Maps right-hand side of linear system on h-grid onto right-hand side on $2h$-grid
  (Haven't needed that so far, as we assumed that b_h is known for all h))

Multigrids (3)

- Restriction can be obtained by simply omitting every second grid point
- Other choice: *weighted restriction*

$$R_h^{2h} := \frac{1}{4} \begin{pmatrix} 1 & 2 & 1 & & & & \\ & & 1 & 2 & 1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & 1 & 2 & 1 \end{pmatrix}$$



- Remark: The property $R_h^{2h} = c \cdot \left(I_{2h}^h\right)^T$ (provided by weighted restriction) is sometimes helpful, especially concerning the analysis of such schemes

Multigrids (4)

- We now have assembled everything for *coarse grid correction*:
  - Compute on fine grid residual $r_h = b_h - A_h x_h$ for current iterated x_h
  - Transport to coarse grid: $r_{2h} = R_h^{2h} r_h$
  - Solve (approximately) $A_{2h}(-e_{2h}) = r_{2h}$
  - Transport correction to fine grid and apply to current iterate: $x_h^{new} := x_h + I_{2h}^h(-e_{2h})$
- Additionally, we have to treat the high frequencies
  - For example, by some steps of a damped Jacobi method which we call *smoother*
  - Doesn't necessarily reduce error, but smooths them as high frequencies are eliminated

Multigrids (5)

- In the example problem, the eigen values of the iteration matrix suggest to damp as high-frequency error components oscillate so much that they are practically not reduced
- With, e.g., $\alpha = 1/2$ we can overcome this
- On $2h$-grid we typically don't solve linear system exactly
- Instead: apply idea of coarse grid correction recursively
- Recursion stops if h is so large that obtaining exact solution is cheap or – for $h = 1/2$, e.g. – trivial
- We thus assume that m is power of two
- As we compute $-e_{2h}$ iteratively, we need initial value; zero vector is best choice due to several reasons...

Multigrid Algorithm

- We have two yet unknown parameters in our algorithm:
- The numbers $\nu_1, \nu_2, \mu \in \mathbb{N}$ denote the number of smoothing steps before and after the coarse grid correction, and the number of recursive calls within coarse grid correction:

$mg(x_h, b_h, \nu_1, \nu_2, \mu)$:

if $h = 2^{-l_{min}}$

solve $A_h x_h = b_h$ exactly

else

Pre-smoothing:

Apply ν_1 smoothing steps to $A_h x_h = b_h$

Coarse grid correction:

for $k = 1, \ldots, \mu$:

$x_h := x_h + I_{2h}^h(mg(0_{2h}, R_h^{2h}(b_h - A_h x_h), \nu_1, \nu_2, \mu))$

Post-smoothing:

Apply ν_2 smoothing steps to $A_h x_h = b_h$

end if

Effort/Cost

How does it look like for the effort?

- Consider the application of I_{2h}^{h} and R_{h}^{2h} to be about as expensive as one smoothing steps
- This is realistic: we have to evaluate a local stencil for the fine grid

$\Rightarrow$ The effort with N grid points is about

$$C \cdot M \cdot (\nu_1 + \nu_2 + 2\mu)$$

plus effort for μ coarse grid corrections

- C is cost per grid point (small, constant number of operations)

Effort/Cost (2)

Cost for coarse grid points

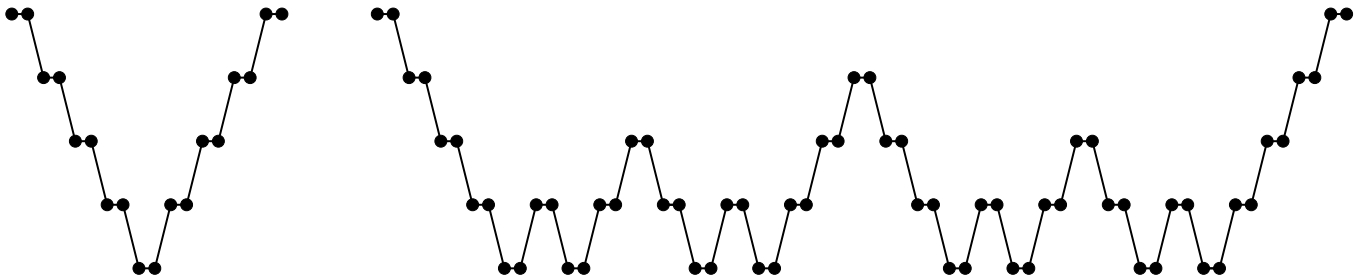
- One-dimensional model problem (as considered):
  - Smoothness and grid transfer costs for $2h$-grid are half as high as for h-grid
  - For $\mu = 1$ the total cost is about

$$1 + 1/2 + 1/4 + \ldots = 2$$

    times the cost on fine grid, i.e., proportional to number of grid points (on finest grid)
  - For $\mu = 2$ the cost per grid point grows logarithmically in M
- Problem transferred to two or three spatial dimensions:
  - Calculation looks even much better:
  - On all coarse grids together there are just $1/3$ ($2d$), or $1/7$ ($3d$) respectively, as many grid points as on finest grid
  - There, even for $\mu < 4$ and $\mu = 8$ we obtain overall effort proportional to number of unknowns on fine grid

Effort/Cost (3)

- Typical choices: $\mu = 1$ (V-cycle), and $\mu = 2$ (W-cycle)



Effort/Cost (4)

- We do not recompute, but just notice (and verify experimentally?) the other part of efficiency considerations:
  - Convergence rate (for $\nu_1 = \nu_1 = \mu = 1$, e.g.) is bounded by 1 independent of fine grid mesh-width h
- Typical multigrid convergence rates for well-behaved problems are about $1/2$ and smaller

$\Rightarrow$ We need only few steps to obtain small error

Hierarchical Methods...

Summary

Hierarchical are beneficial in many settings

- Can allow to reduce cost
- Can allow to "compress" functions (represent with few degrees of freedom)
- Can allow to estimate errors
- Can provide "level of detail" (coarse partial solutions)
- Can allow to compute coarse approximations
- Can be used to define refinement criteria
- Can speed up the solution of linear systems
- ...