Algorithms, Implementation and Applications of pFFT++:

Direct matrix, pre-correction and grid selection

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Outline

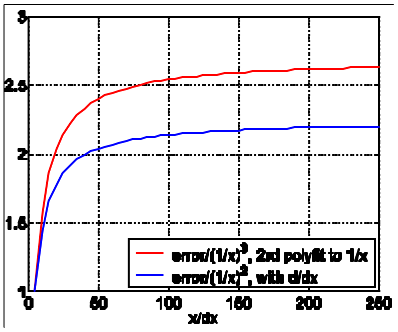
- Derivation of interpolation error bound
- How to find nearby neighbors
- Pre-correction
- Grid selection
- Implementation details

How to find nearby neighbors: derivation of error bound

- 1D interpolation
- 3D interpolation (optional)

<u>All shown with chalk and board</u>

How to find nearby neighbors: error bound for double-layer (1D)



How to find nearby neighbors: interpolation error bound

If a panel is within the region covered by the stencil, leading term in relative error is

$$e \approx \left(\frac{h}{r_0}\right)^{n+1}$$

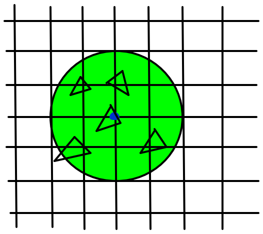
If some part of a panel hang out of the region covered by the stencil, leading term in relative error is

$$e \approx \left(\frac{a}{r_0}\right)^{n+1}$$

where a is the radius of the panel

How to find nearby neighbors: basic strategy

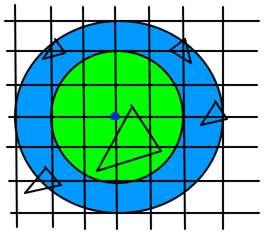
- For regular panels
  - Use direct stencil (sphere shape) as metric to find nearby neighbors



- Go through each point in the direct stencil and find the panels mapped to the point
- Add these panels to the <u>regular neighbor list</u>

How to find nearby neighbors: basic strategy

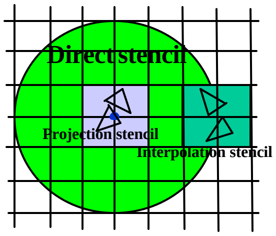
- For large panels
  - Measure physical distance against the radius of the panels



- Find all grid points a certain distance from stencil center
- Exclude all direct stencil points and find the panels mapped to the remaining points
- Add these panels to the irregular neighbor list

Pre-correction: regular neighbors

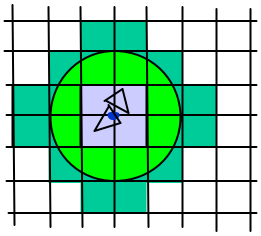
$$D_{i,j} = D_{i,j} - \left[I_i \right]_{1\times9} \left[H \right]_{9\times9} \left[P_j \right]_{9\times1}$$



- Find an interpolation stencil center around each direct stencil point
- Fill in a small convolution matrix [*H*]
- Pick appropriate row and column of [I] and [P], calculate the pre-correction
- Pre-correct the appropriate entry in [*D*]

Pre-correction: improvement on regular neighbors

$$D_{i,j} = D_{i,j} - \left[I_i \right]_{1\times9} \left[H \right]_{37\times9} \left[P_j \right]_{9\times1}$$



- Find the union of the interpolation stencil center around each direct stencil point (37 points in this figure)
- Fill in a long skinny convolution matrix [*H*]
- Pick appropriate column of [P], calculate [*g*] = [*H*] [*P*]
- Pick appropriate row in [*I*] and [*g*], calculate [*I*][*g*]
- Pre-correct the appropriate entry in [*D*]

Pre-correction: improvement on regular neighbors

- **Before:** $\left[H \right]_{9\times9} \left[P_j \right]_{9\times1}$

repeat *n* time, *n* being number of points in direct stencil

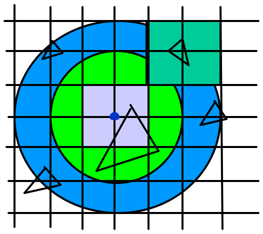
- **After:** $\left[H \right]_{37\times9} \left[P_j \right]_{9\times1}$

Do it just once. Keeping track of index may add some overhead cost.

- **Key: interpolation stencils share grid points**

Pre-correction: irregular neighbors

$$D_{i,j} = D_{i,j} - \left[I_i \right]_{1\times9} \left[H \right]_{9\times9} \left[P_j \right]_{9\times1}$$



- Find the interpolation stencil for each irregular neighbor
- Fill in a small convolution matrix [*H*]
- Pick appropriate row and column of [I] and [P], calculate the pre-correction
- Pre-correct the appropriate entry in [*D*]

Grid selection: minimize memory usage

- Once the grid size satisfies certain constrains with respect to the element size, the accuracy is decided by the error bound.
- Larger number of grid points leads to larger memory usage by [*H*], but [*D*], [*I*] and [*P*] would be sparser.
- There is an optimal grid size that balance these two factors.

Grid selection: An optimization problem

Minimize memory usage by [*I*], [*P*], [*D*] and [*H*] Subject to

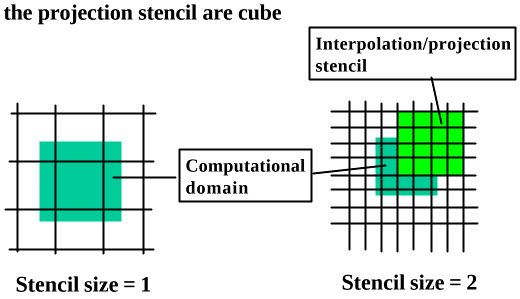
1. **reasonable ratio between grid size and element size, no extrapolation.**
2. **grid size is smaller than a tenth of a wavelength if the kernel is oscillatory.**
3. **not too many elements associated with one grid point.**
4. **Minimize size of the region occupied by grid.**
5. **Number of grids is 2^n**

Grid selection: An optimization problem

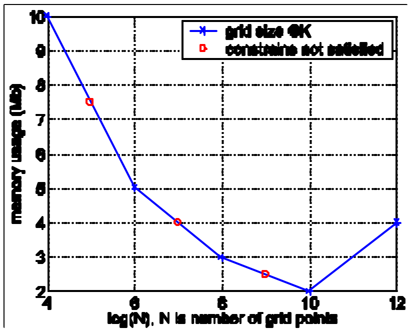
- **Ultimate test is the memory usage**
- **Constrains are used to weed out a grid option cheaply**
- **To gauge memory usage, grid and element map is to be set up.**
- **Density and size of [*I*], [*P*], [*D*] and [*H*] can be easily derived from grid element map. Hence memory estimation itself is cheap.**
- **There is not guarantee that a legitimate grid can be found, particularly for long and thin panels.**

Grid selection: starting point

Need extra layers to ensure that the interpolation and the projection stencil are cube



Grid selection: typical search pattern



Implementation: Source codes

- **See gridElement.cc for how to find the nearby neighbors**
- **See directMat.h and g2gUnion.h for pre-correction details**
- **See grid.cc for grid selection**

Next Lecture

- **High-order element in pfft**
- **Application of pfft++ in computational aerodynamics**