Algorithms, Implementation and Applications of pFFT++:

More on projection and interpolation

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Outline

- Error bound
- Loss of accuracy in double-layer potential
- Consistent polynomials
- Compact stencil
- Selection of three stencil sizes
- Implementation details

1D polynomial fit

Suppose the function is

$$f(x) = \frac{1}{x}$$

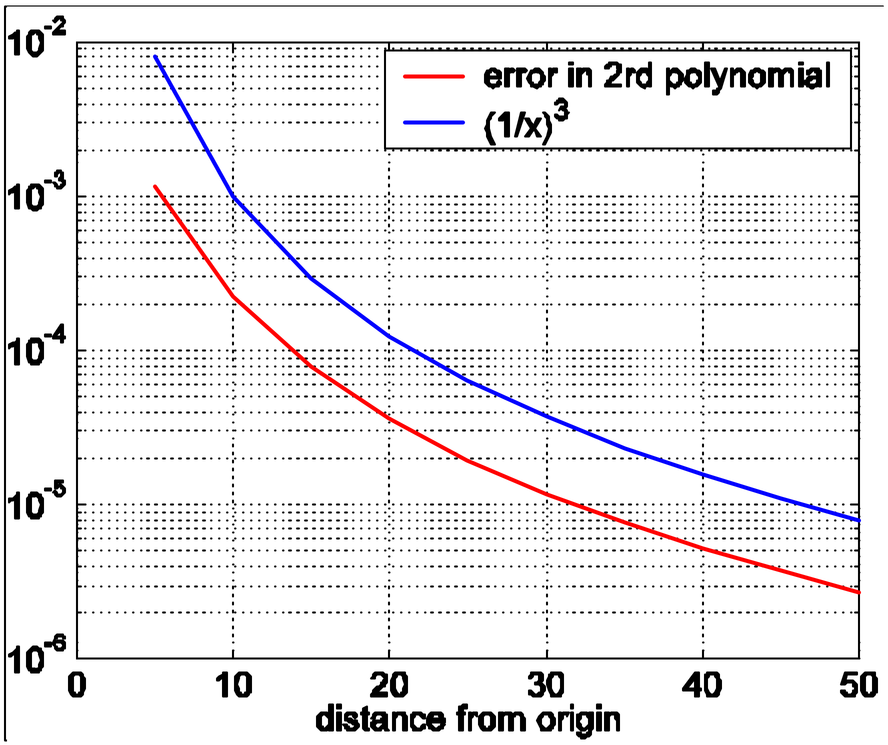
Using a second-order polynomial to interpolate around x_0, the relative error is

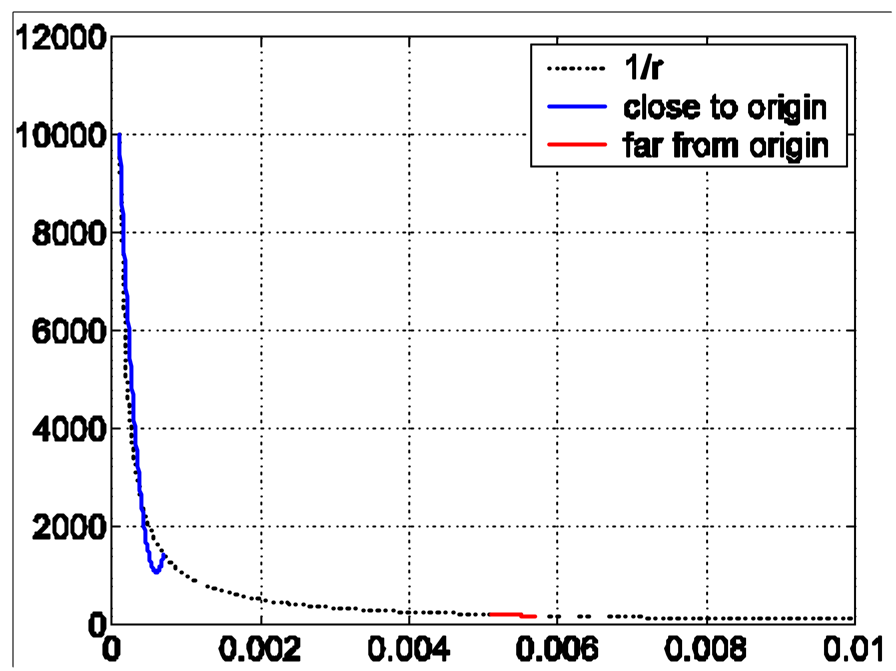
$$e \approx \left(\frac{h}{x_0} \right)^3$$

where h is the uniform grid spacing.

See "Introduction to numerical analysis" by Stoer and Bulirsch

1D polynomial fit





Error bound in pfft++:

Two factors in determining the error:

1. **Direct stencil size**

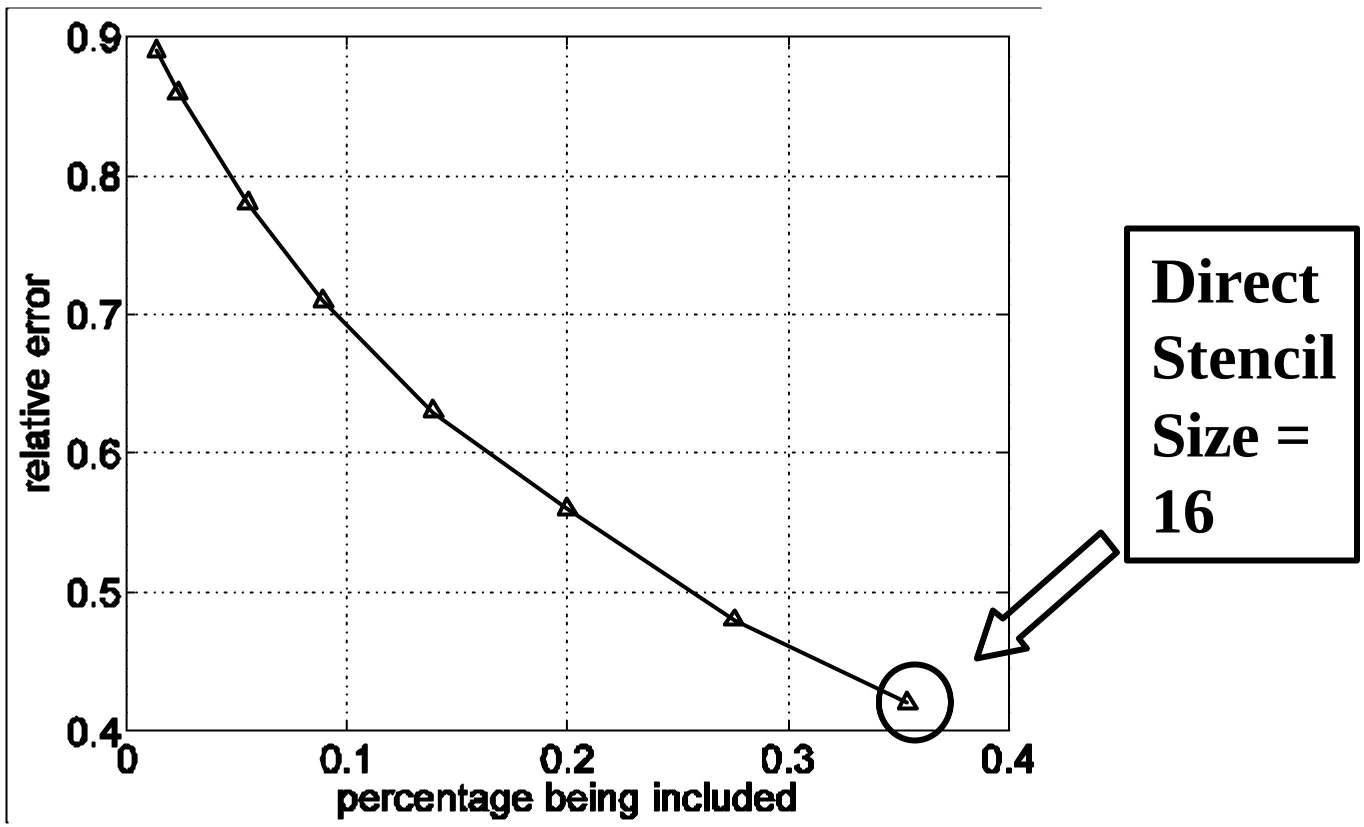
   Larger size means more interactions are calculated directly and larger distance to non-neighbor elements.

2. **Interpolation and projection size**

   Higher order means lower interpolation error.

Error bound in pfft++: Truncation error

Suppose we only keep the direct interaction and ignore far field completely, i.e. let $[A] = [D]$. We effectively truncate the system matrix.



Error bound in pfft++: 3D interpolation error

Given (x_l, y_l, z_l) and $f_l = f(x_l, y_l, z_l)$, use *n*-th order polynomial to approximate $f(x,y,z)$

$$P_n(x,y,z) = \sum_{m=0}^{n} \sum_{i=0}^{m} \sum_{j=0}^{m-i} C_{ij} x^i y^j z^{m-i-j}$$

Let

$$F(x,y,z) = f(x,y,z) - P_n(x,y,z) - w_{n+1}(x,y,z)$$

where

$$w_{n+1}(x,y,z) = \sum_{i=0}^{n+1} \sum_{j=0}^{n+1-i} k_{ij} (x - x_l)^i (y - y_l)^j (z - z_l)^{n+1-i-j}$$

is the leading error term

Error bound in pfft++:
3D interpolation error

For 1/r kernel, the leading term in error is

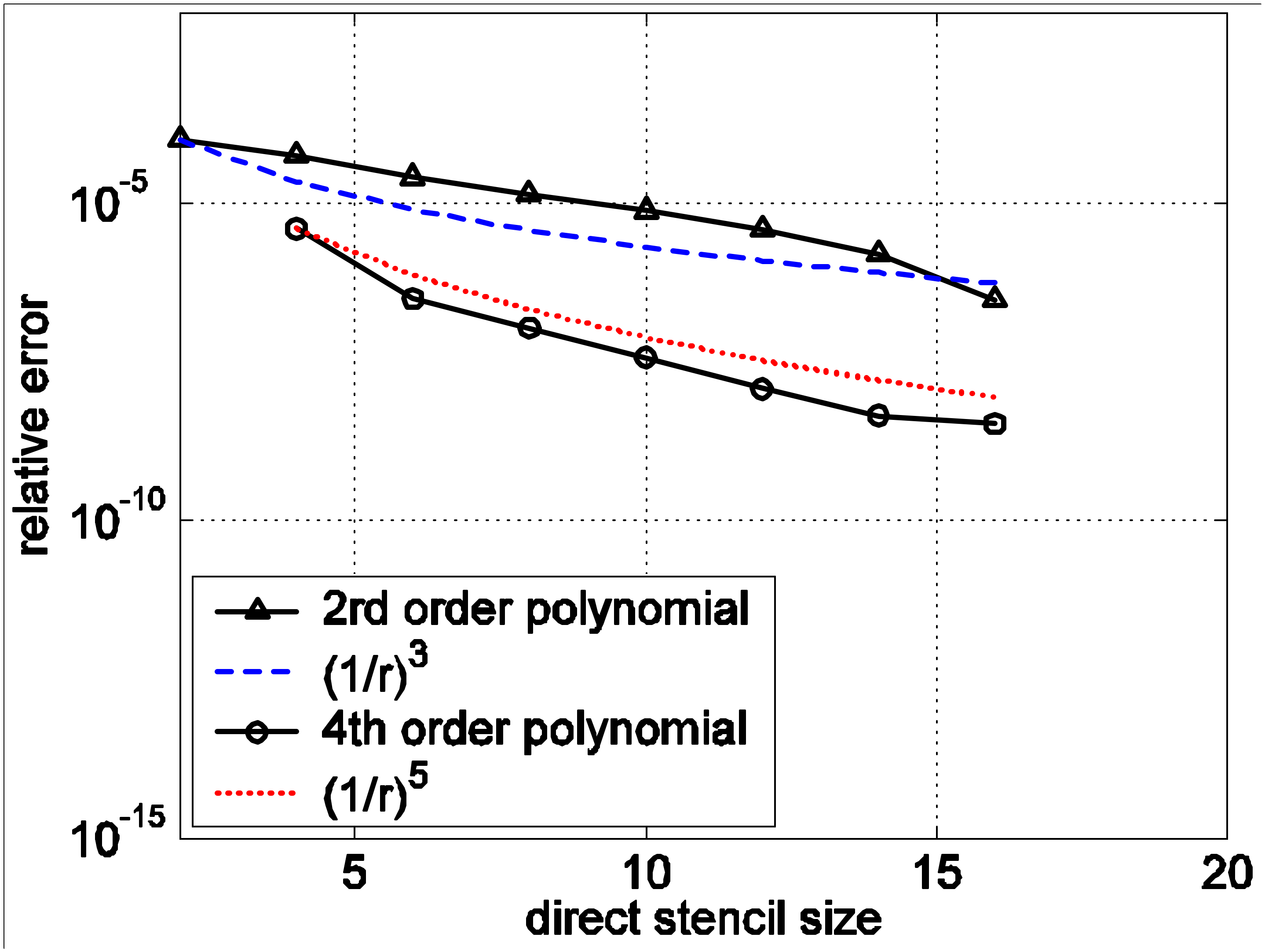
$$\frac{1}{r}\left(\frac{h}{r}\right)^{n+1}\sum_{i=0}^{n+1}\sum_{j=0}^{n+1-i}\left(\frac{\partial r}{\partial x}\right)^{i}\left(\frac{\partial r}{\partial y}\right)^{j}\left(\frac{\partial r}{\partial z}\right)^{n+1-i-j}$$

So the relative error is $e \approx \left(\frac{h}{r_0}\right)^{n+1}$

where *h* is the uniform grid spacing and r_0 is the distance between the source and the evaluation point.

<u>**Derivation shown with chalk and board**</u>

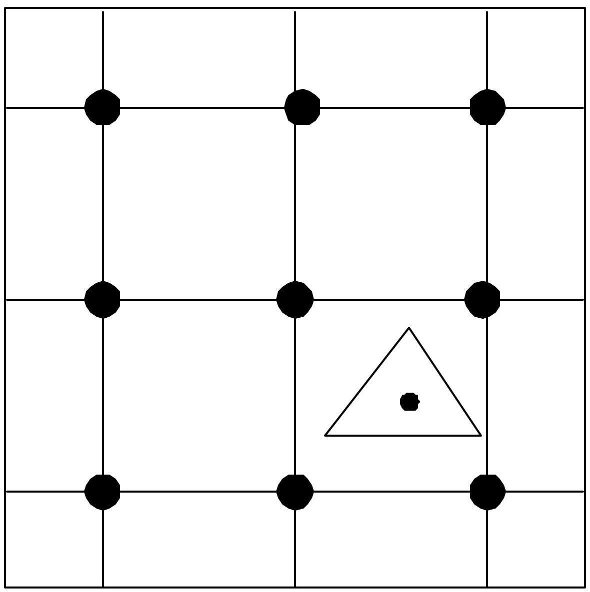
Error bound in pfft++



Loss of Accuracy in double-layer potential

	$P = 3$	$P = 5$	$P = 7$
$1/r$	8.4e-5	1.3e-6	4.3e-9
$\frac{\partial}{\partial n} 1/r$	8.5e-3	1.1e-4	8.4e-7
e^{ikr}/r *kR* = 1.1e-9	8.3e-5	1.3e-6	1.7e-9
$\frac{\partial}{\partial n} e^{ikr}/r$ *kR* = 1.1e-9	6.0e-3	7.5e-5	5.9e-7
e^{ikr}/r *kR* = 11.1	4.9e-4	1.1e-5	4.0e-7
$\frac{\partial}{\partial n} e^{ikr}/r$ *kR* = 11.1	1.4e-2	2.8e-4	6.5e-6

Reminder of Interpolation Algorithm



Given $\bar{f}_g$

Compute $f(x, y)$

Reminder of Interpolation Algorithm

$$f(x,y) = \sum_k c_k f_k(x,y) = \overline{f}^t(x,y)\overline{c}$$

An example of $f_k(x,y)$:

$$1, x, x^2, y, xy, x^2y, y^2, xy^2, x^2y^2$$

Reminder of Interpolation Algorithm

If the kernel has a differential operator outside:

$$\frac{\partial}{\partial n(\vec{r})}\int_S dS' G(\vec{r},\vec{r}')r(\vec{r}')$$

The operator works on the interpolation

$$\frac{\partial}{\partial n(\vec{r})} f(\vec{r}) = \frac{\partial}{\partial n(\vec{r})}\bar{f}^t(\vec{r})F^{-1}\bar{f}_g$$

Loss of Interpolation Order

$$\frac{\partial \bar{f}^t}{\partial n} = n_x \frac{\partial \bar{f}^t}{\partial x} + n_y \frac{\partial \bar{f}^t}{\partial y}$$

$$\bar{f}^t = 1, x, x^2, y, xy, x^2 y, y^2, y^2 x, y^2 x^2$$

$$\frac{\partial \bar{f}^t}{\partial x} = 0, 1, 2x, 0, y, 2xy, 0, y^2, 2y^2 x$$

$$\frac{\partial \bar{f}^t}{\partial y} = 0, 0, 0, 1, x, x^2, 2y, 2yx, 2yx^2$$

We automatically lose interpolation order.
This is why double-layer is less accurate.

Loss of Interpolation Order

- **Double-layer still has reasonable accuracy because of smoothness of far field.**
- **We can simply increase interpolation order to compensate the loss of degree in derivative**
- **But stencil size grows exponentially**

order	2	4	6
# monomials	27	125	343
# stencil grid points	27	125	343

Consistent Polynomials

Suppose the highest order is *n*, using consistent polynomial, we have

$$f(x, y, z) = \sum_{m=0}^{n} \sum_{i=0}^{m} \sum_{j=0}^{m-i} c_{ijk} x^i y^j z^{m-i-j}$$

$$\text{total number of terms} = (n+1)(n+2)(n+3)/6$$

n	2	4	6
# monomials	10	35	84

Compact Stencil

Number of interpolation terms is much fewer than number of regular interpolation or projection stencil points. We have a least square problem

$$\left[F\right]^{-1}_{n_s \times n_p}$$

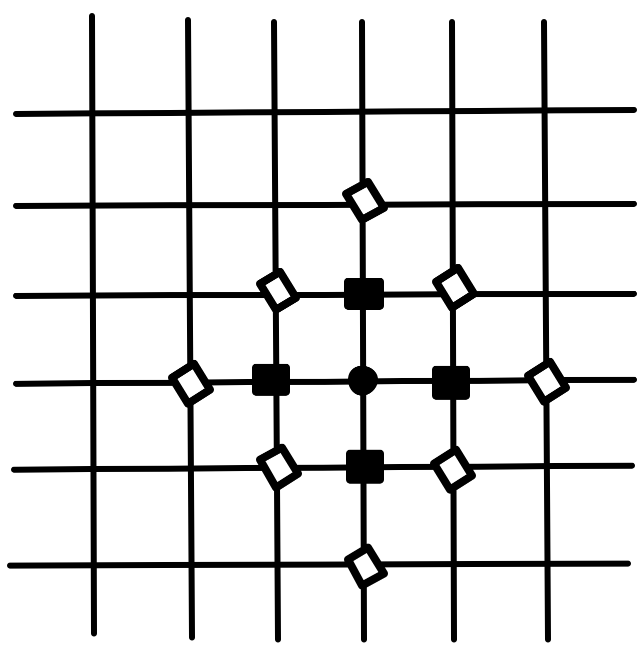
where n_s is number of stencil points and n_p is number of monomials. We could pick points from regular stencil points. Many options are possible.

Compact Stencil:
2D Example

Union of points equal distance from the origin of the interpolation stencil

$$\text{Cube stencil} = S_0 \cup S_1 \cup \frac{1}{2} S_2$$

$$\text{Compact stencil} = S_0 \cup S_1 \cup S_2$$



S_0: 1 solid dot
S_1: 4 solid squares
S_2: 8 empty diamonds

New Interpolation Scheme

- **Same order of accuracy but with much fewer monomials and stencil points.**
- **Particularly useful for high-order interpolation**

order	2	4
# monomials	27	35 (consistent)
# stencil grid points	27	57

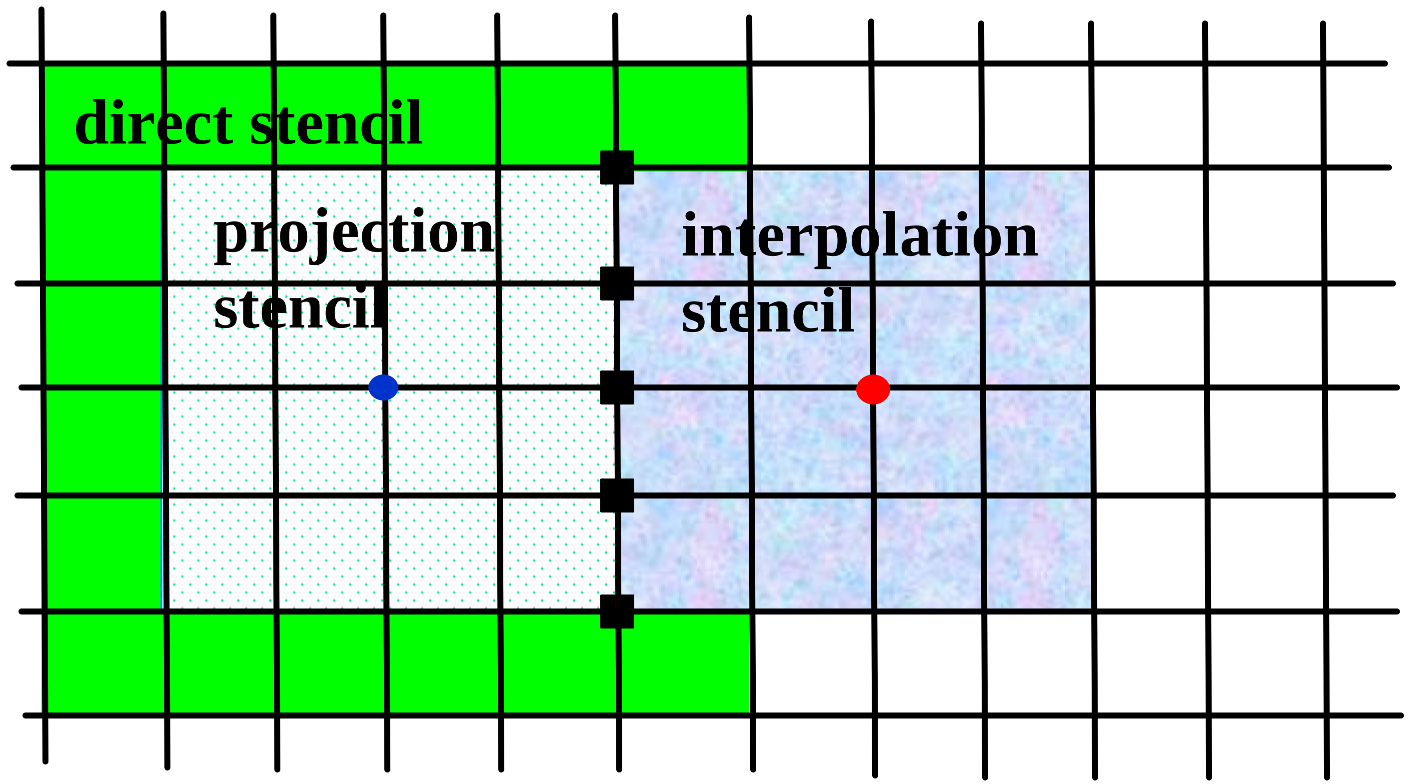
Compact stencil S_{012345} is used here.

Selection of Three Stencil Sizes

- **Increase of direct stencil size is not cost effective**
  - ❑ **accuracy improves slowly**
  - ❑ **density of [*D*] increases relatively fast**
- **Increase of interpolation or projection stencil size improves accuracy exponentially.**
  - ❑ **Consistent polynomial makes the cost low**
- **There exists a constrain on these three stencil sizes.**

Selection of Three Stencil Sizes

■ **points shared by projection and interpolation stencil, corresponding entries in [*H*] are zero!**



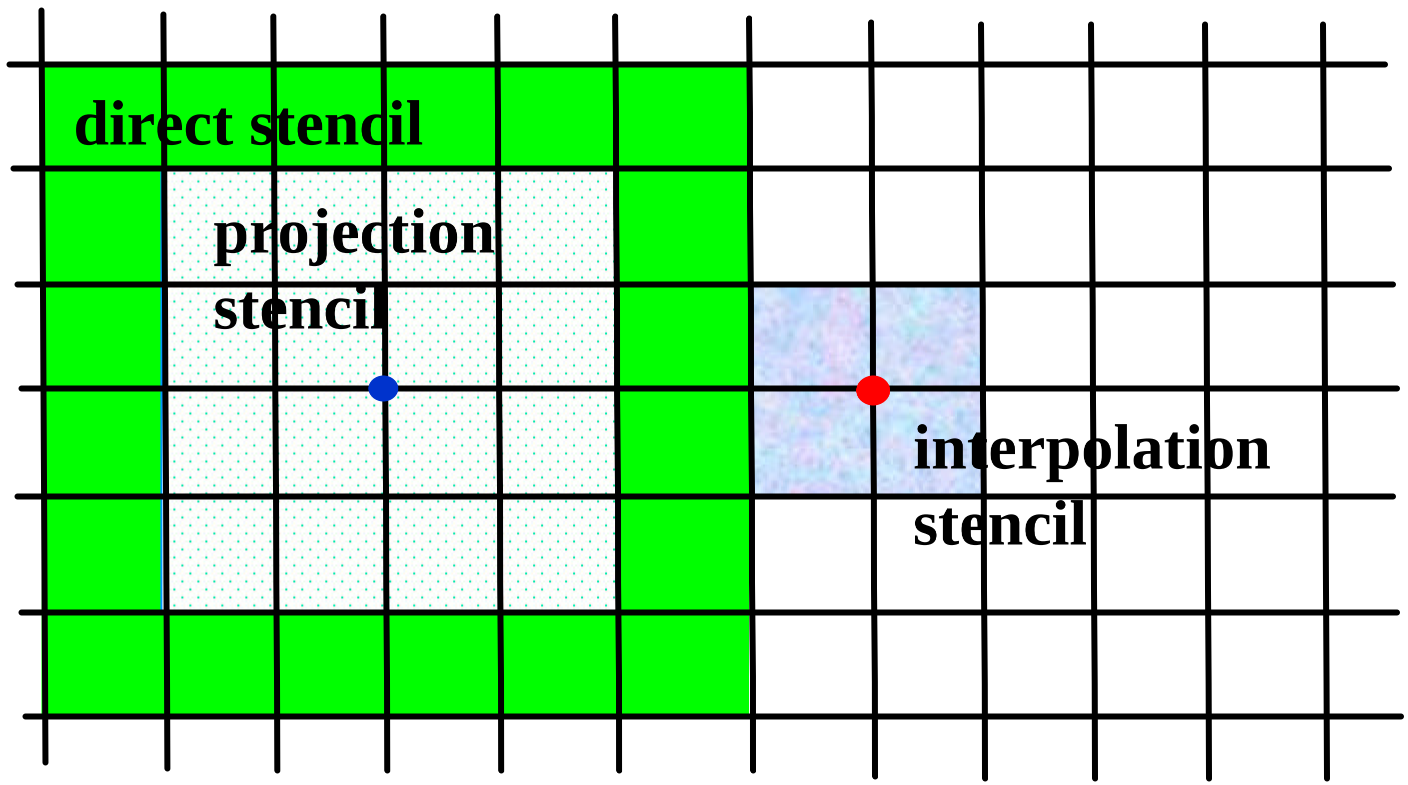
● **Center of direct and projection stencil**

● **Center of interpolation stencil**

Selection of Three Stencil Sizes

To make sure interpolation and projection Stencil don't touch, enforce

directStencilSize >= projectStencilSize + interpStencilSize



Selection of Three Stencil Sizes: rule of thumb

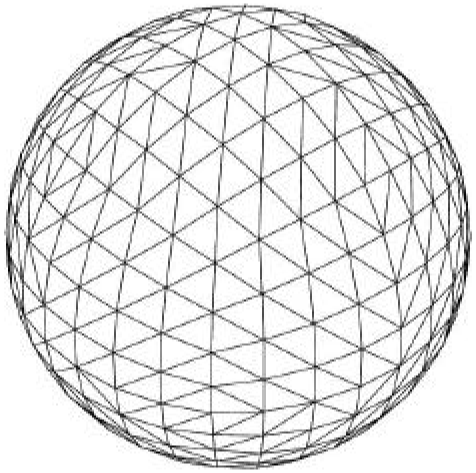
- **Single-layer**
  - **3-4 digit: I=P=1, D=2**
  - **4-5 digit: I=P=1, D=3**
  - **5-6 digit: I=P=2, D=4**
- **Double-layer**
  - **2-3 digit: I=P=1, D=3**
  - **4-5 digit: I=P=2, D=4**
  - **5-6 digit: I=P=2, D=5 or 6**
- **pfft++ supports I=P=3, but try not to use it. It is too costly.**

Numerical Experiments

On the surface of a sphere with radius *R*

$$\int_S dS' K(\vec{r}, \vec{r}')\, r(\vec{r}') \Rightarrow Ax$$

Let *x* be a random vector



$$y_1 = Ax$$

$$y_2 = pfft(x)$$

$$error = \frac{\left\| y_1 - y_2 \right\|_2}{\left\| y_1 \right\|_2}$$

New Accuracy in double-layer potential

	$I=P=1$, D=3	$I=P=2$, D=4 (Consistent poly)
$1/r$	8.4e-5	1.3e-6
$\frac{\partial}{\partial n} 1/r$	8.5e-3	3e-4
e^{ikr}/r ***kR = 11.1***	4.9e-4	1.1e-5
$\frac{\partial}{\partial n} e^{ikr}/r$ ***kR = 11.1***	1.4e-2	6.2e-4

Implementation:
Source codes

- See stencil.cc
- See pfft.h

Next Lecture

- **Direct matrix and pre-correction**
- **Grid selection**