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Multi-Shifted Bi-Conjugate Gradient Stabilized

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In this note, I describe how to use the multi-shifted bi-conjugate gradient stabilized (BICGStabM) for the inversion of linear systems involving the wilson fermionic matrix for several values of κ .

In the following, we are interested in inverting the linear system

$$(\mathbf{1} - \kappa \mathcal{D}) \mathbf{x} = \mathbf{b}. \quad (1)$$

We first have to cast it into the shifted form

$$(M + \sigma) \mathbf{x} = \mathbf{b} \quad (2)$$

This can be achieved with the following definitions

$$\mathbf{x}' = -\mathbf{x}/\kappa \quad \sigma = -\frac{1}{\kappa} \quad M = \mathcal{D} \quad (3)$$

which written explicitly is

$$[\mathcal{D} + (-1/\kappa)] (-\kappa \mathbf{x}) = \mathbf{b} \quad (4)$$

Therefore, we can solve for the solutions \mathbf{x}' and recover the original solution $\mathbf{x} = -\mathbf{x}'/\kappa$ by a simple rescaling.

To use the BICGStabM, we pass the most singular shifted matrix — the one that takes the most iterations. The algorithm then iterates until *this* system converges to the desired accuracy and exits. Since this is the most singular shifted matrix, all other solutions should have converged. **Note: The algorithm does not check this for you. You need to check this in your code.**

In the following, will work through a concrete example. Let's assume we have a three κ values. $\text{shifts} = \{\kappa_0, \kappa_1, \kappa_2\}$ and κ_0 is the most singular one. For the wilson fermionic matrix, this corresponds to the largest value of κ . The function call is given by

```
int qcd::bicgstabm_device(  
device_wilson_field &src, int noshifts, double shifts[],  
device_wilson_field *sol[], double dError,  
int maxiters, matmult<device_wilson_field>& pfncMatMult,  
device_random_field& rnd  
);
```

- define the matrix multiplication to be $\text{pfncMatMult} = \mathcal{D} - 1/\kappa_0$

- define the remaining two shifts as $\sigma_i = 1/\kappa_0 - 1/\kappa_i$ $i = 1, 2$ so that

$$M + \sigma_i = \not{D} - 1/\kappa_0 + 1/\kappa_0 - 1/\kappa_i = \not{D} + (-1/\kappa_i) \quad (5)$$

which is the desired result (see eq. ??).

- set shfits = $\{\sigma_1, \sigma_2\}$.
- set noshifts = 2.
- set src = **b**.
- I set dError = 1e-10.
- pass an array of 3 pointers to device_wilson_fields.
- set the maxiters accordingly and pass an instance of a device_random_field for rnd.
- the results are stored in sol where *sol[i] is the solution for the i^{th} κ .
- Lastly rescale the solutions accordingly.