Conjugate Gradient Solver for SU(2) Staggered Fermion on GPU

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Outline

Motivation
Staggered Fermion
Conjugate Gradient Solver
GPU Computation
Example
Summary and Comments

Motivation

SU(2) Gauge Theory with many flavor
= Candidate of Beyond Standard Model
(Walking Techni-Color)

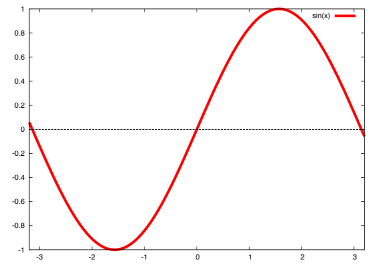
Strongly Interacting System
=> Lattice Simulation is useful tool

HMC Simulation & Measurement
=> Need to Solve Linear Equation $s = Dx$ (x is unknown)
Conjugate Gradient or it's modification is widely used.

GPU is effective for sparse matrix calculation

Staggered Fermion

Way out of Nielsen Ninomiya No-go theorem



$$S_F = \frac{1}{2}\sum_{n,\mu}\eta_\mu(n)\left[\bar{\chi}(n)U_\mu(n)\chi(n+\hat{\mu}) - \bar{\chi}(n)U^\dagger_\mu(n-\hat{\mu})\chi(n-\hat{\mu})\right] + M\sum_n \bar{\chi}(n)\chi(n)$$

$$\eta_\mu(n) = (-1)^{n_1+n_2+\cdots+n_{\mu-1}}$$

=>

$$S_F = \frac{1}{2}\sum_{n,\mu}\left[\bar{\chi}(n)U'_\mu(n)\chi(n+\hat{\mu}) - \bar{\chi}(n)U'^\dagger_\mu(n-\hat{\mu})\chi(n-\hat{\mu})\right] + M\sum_n \bar{\chi}(n)\chi(n)$$

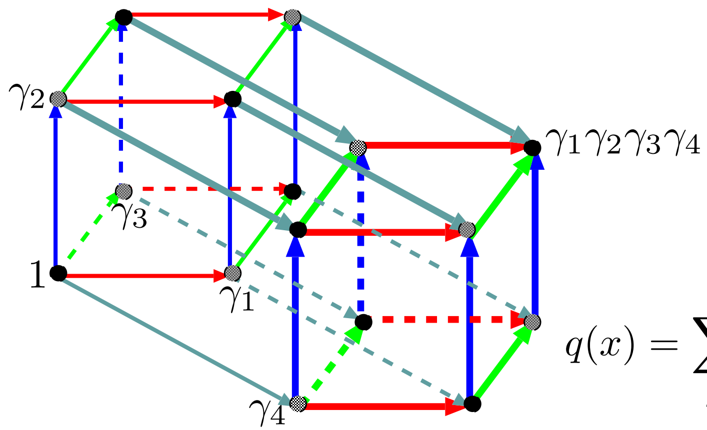
$$U'_\mu(n) = \eta_\mu(n)U_\mu(n)$$

Hyper Cube (16 DOF)

=>

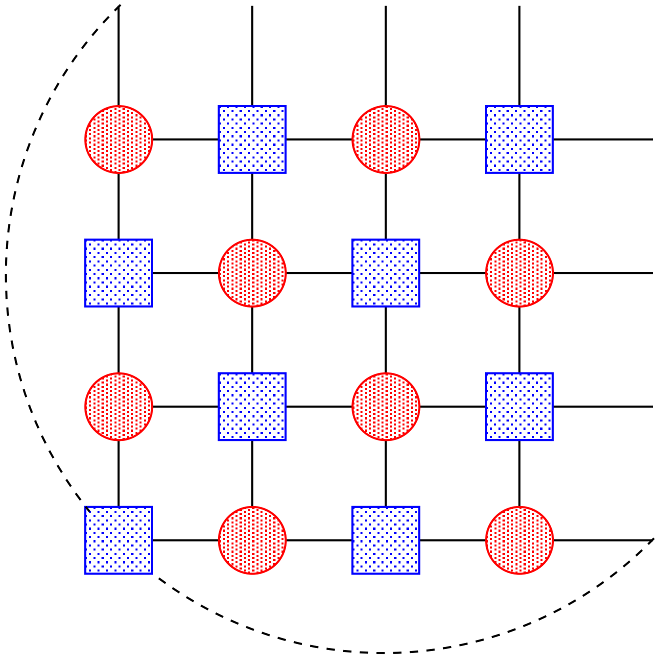
Considered as 4 dirac

and “4 taste”



$$q(x) = \sum_{\rho_i}\gamma^{\rho_1}\gamma^{\rho_2}\gamma^{\rho_3}\gamma^{\rho_4}\chi(x+\rho)$$

Even-Odd Preconditioning (Checkerboard)



Even Site:

(ix + iy + iz + it) % 2 =0

$$\begin{pmatrix} m & D_{EO} \\ D_{OE} & m \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ D_{OE}\frac{1}{m} & 1 \end{pmatrix} \begin{pmatrix} m & 0 \\ 0 & m - D_{OE}\frac{1}{m}D_{EO} \end{pmatrix} \begin{pmatrix} 1 & D_{EO} \\ 0 & 1 \end{pmatrix}$$

Inverse

$$\begin{pmatrix} m & D_{EO} \\ D_{OE} & m \end{pmatrix}^{-1} = \begin{pmatrix} 1 & -D_{EO} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} m & 0 \\ 0 & \boxed{m - D_{OE}\frac{1}{m}D_{EO}} \end{pmatrix}^{-1} \begin{pmatrix} 1 & 0 \\ -D_{OE}\frac{1}{m} & 1 \end{pmatrix}$$

Determinant

$$\det \begin{pmatrix} m & D_{EO} \\ D_{OE} & m \end{pmatrix} = \det \begin{pmatrix} m & 0 \\ 0 & \boxed{m - D_{OE}\frac{1}{m}D_{EO}} \end{pmatrix}$$

Conjugate Gradient $b = Ax$

Initial Condition

$$d_0 = r_0 = b - Ax_0$$

Iteration i=0,1,2, ...

$$x_{i+1} = x_i + \alpha_i d_i$$ .... 2 Solution

$$d_{i+1} = r_{i+1} + \beta_{i+1} d_i$$ .... 5 Update Direction

$$r_{i+1} = r_i - \alpha_i A d_i$$ .... 3 Residual

Coefficients are

$$\alpha_i = \frac{(r_i, r_i)}{(d_i, Ad_i)}$$ 1

$$\beta_{i+1} = \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)}$$ 4

Conjugate Gradient $b = Ax$

Initial Condition

$$d_0 = r_0 = b - Ax_0$$

Iteration i=0,1,2, ...

$$\alpha_i = \frac{(r_i, r_i)}{(d_i, Ad_i)}$$

$$r_{i+1} = r_i - \alpha_i A d_i$$ Residual

$$x_{i+1} = x_i + \alpha_i d_i$$ Solution

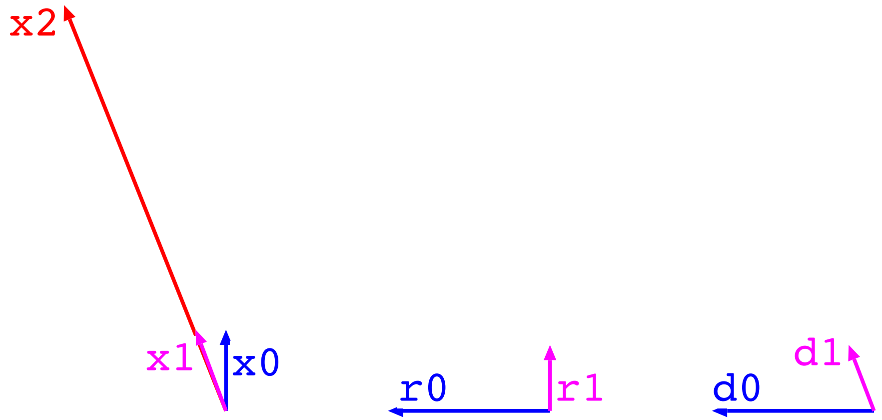
$$\beta_{i+1} = \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)}$$

$$d_{i+1} = r_{i+1} + \beta_{i+1} d_i$$ Update Direction

Example $b = Ax$ with $A = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ $b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$d_0 = r_0 = b - Ax_0 \qquad \alpha_i = \frac{(r_i, r_i)}{(d_i, Ad_i)} \qquad x_{i+1} = x_i + \alpha_i d_i$$

$$r_{i+1} = r_i - \alpha_i A d_i \quad \beta_{i+1} = \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)} \qquad d_{i+1} = r_{i+1} + \beta_{i+1} d_i$$



$$(d_i, r_j) = 0 \;\; \text{for } i < j \qquad (r_i, r_j) = 0 \;\; \text{for } i \neq j$$

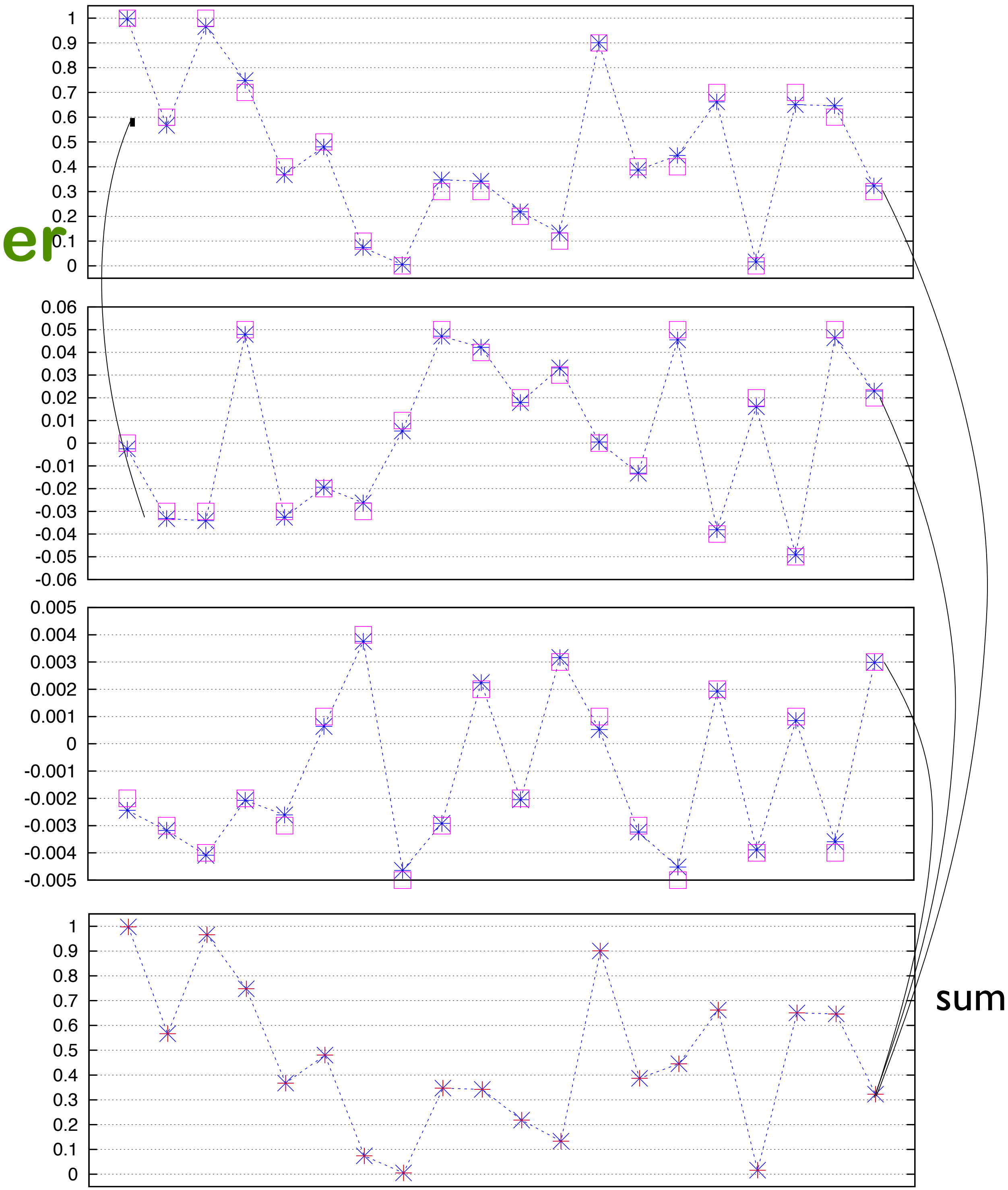
This guarantees $r_N = 0$

Comments on b=Ax

It needs efforts to find the solution.
On the other hand,
It is very easy to check the solution.

This property is crucial for Mixed Precision CG

Concept of Mixed Precision Solver



difference of star and square of above

difference of star and square of above

sum of square

Defect Correction and Reliable Update

Defect Correction

SP: CG Solver, with $d_0 = r_0$

DP: Sum SP solution to DP solution

DP: Calculate residual vector and set it as SP source

$(d_i, r_j) = 0 \quad \text{for } i < j$ Is reset in defect correction

Reliable Update

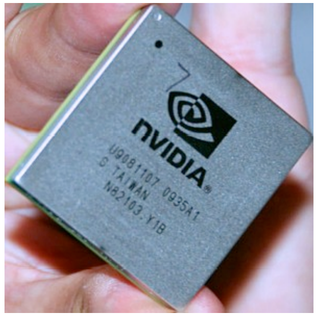
SP: CG Solver, without refreshing d_0

DP: Sum SP solution to DP solution

DP: Calculate residual vector and set it as SP source

Convergence is faster for Reliable Update

GPU (Graphic Processor Units)



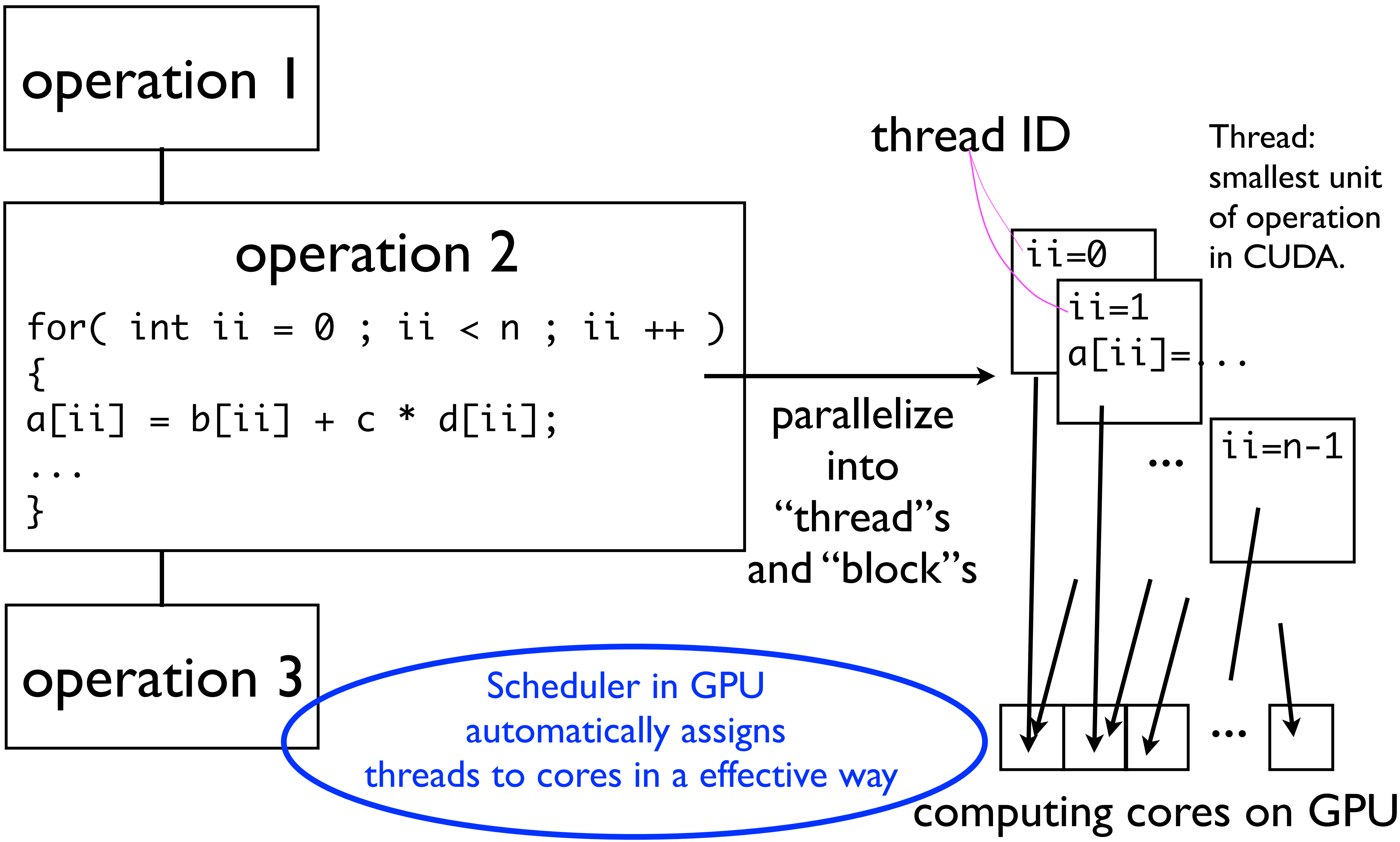
Originally Developed for Video Gamers

many core (~1000) works for SIMD
(Single Instruction Multiple Data) simultaneously

Nvidia's recent product have several level of memory
with different size and access time to the computing cores

Coding with CUDA

CPU Code



Tuning of GPU

Principle = Let processors works all time.
=> reduce the time to get / send data

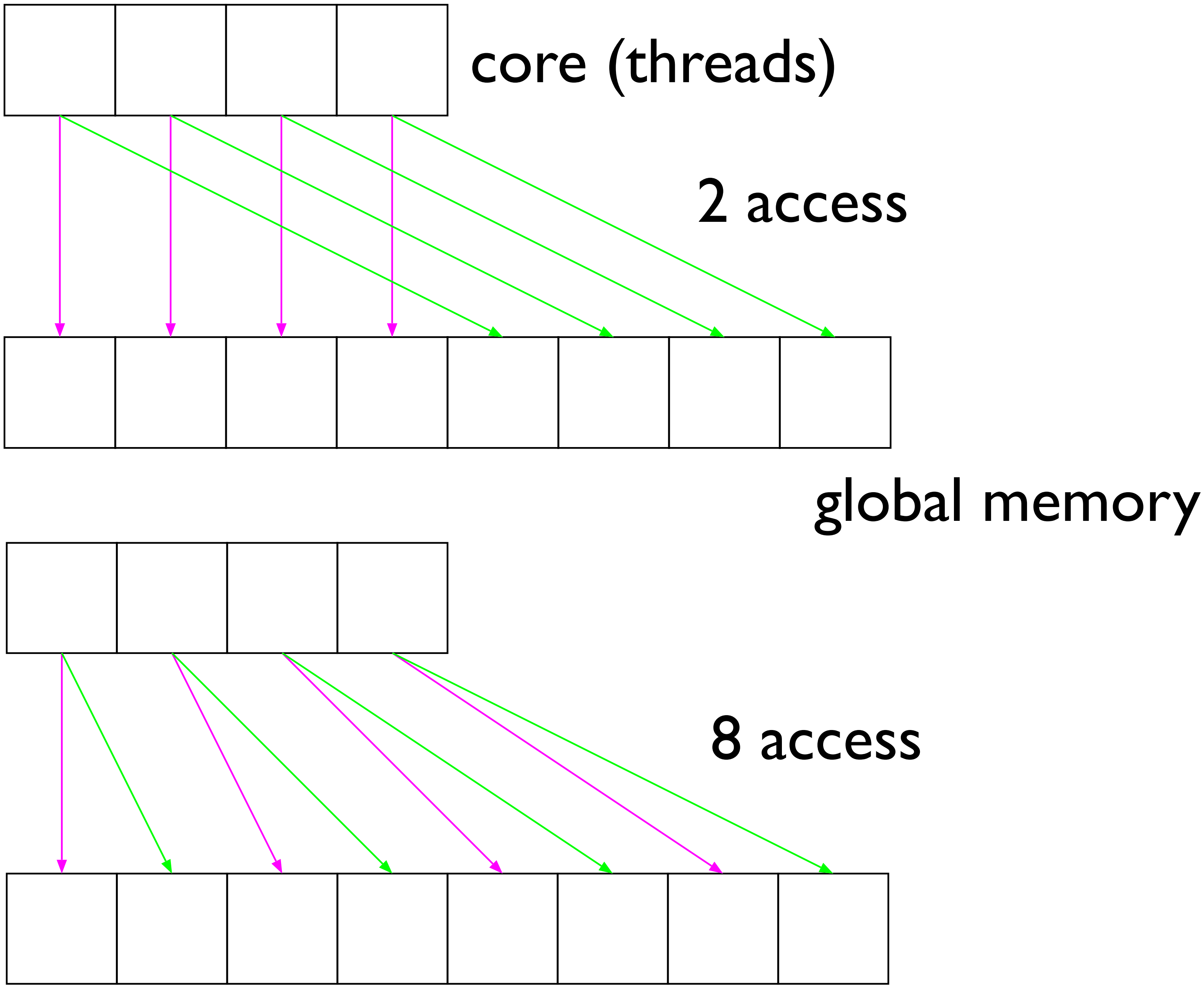
Memory
Turn on/off L1 Cache, Texture, Shared Memory

Coallese
Reorder the data as GPU friendly

Magic Number (depend on the architecture)
Warp, Block Size, ...

Reordering the Operation
Recycle the data on the cache as much as possible

Coallece



Example of Mixed Precision CG

L24^3T48 Lattice, Beta=2.7 , aM = 0.25, Naive Staggered

"Tesla" is used

100 SP Iteration

```
=== DOUBLE PRECISION ===
----- (vR,vR)/(vSrc,vSrc):   1.00000000E+00
=== CG SINGLE PRECISION ===
----- S, T, U :   3.05123917E+09    2.17739184E+08    1.60231230E+07
----- S, T, U :   2.67133362E+02    3.03177528E+01    8.18141556E+00
=== DOUBLE PRECISION ===
----- (vR,vR)/(vSrc,vSrc):   3.75744317E-08
=== CG SINGLE PRECISION ===
----- S, T, U :   9.14439850E+01    8.18142605E+00    2.74593925E+00
----- S, T, U :   2.68391886E-04    2.98086998E-05    7.48642242E-06
=== DOUBLE PRECISION ===
----- (vR,vR)/(vSrc,vSrc):   3.43825294E-14
=== CG SINGLE PRECISION ===
----- S, T, U :   8.44834140E-05    7.48642378E-06    2.51462211E-06
----- S, T, U :   3.13231913E-10    3.60102989E-11    1.46738698E-11
=== DOUBLE PRECISION ===
----- (vR,vR)/(vSrc,vSrc):   6.73919755E-20
=== CG SINGLE PRECISION ===
----- S, T, U :   1.67335437E-10    1.46738732E-11    4.63271088E-12
----- S, T, U :   4.74928462E-16    5.84574362E-17    3.02788868E-17
=== DOUBLE PRECISION ===
----- (vR,vR)/(vSrc,vSrc):   1.39060504E-25
=== MIXED PRECISION CG CONVERGED ===
 Time-CG[sec]   1.340796
```

S, T, U columns annotated: (d_i, Ad_i) (r_{i-1}, r_{i-1}) (r_i, r_i)

Summary and Comments

SU(2) gauge theory
=> Candidate of Beyond Standard Moded

Lattice Simulation
=> Large Part is Solving Linear Problem of Dirac Operator

Speed up of Conjugate Gradient
Even Odd Preconditioning
Mixed Precision
Defect Correction, Reliable Update

1 GPU ~ 1 Node of Super Computer

Special Thanks, Aoyama-san (KMI)