# Multigrid solver for clover fermions

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# Outline

- Multigrid intro
- Adaptive multigrid
- Application to Wilson Clover
- Results
- Setup cost
- Plans

# The problem

- Lattice QCD requires repeated solution of Dirac equation

$$[D(U) + m]\psi = \eta$$

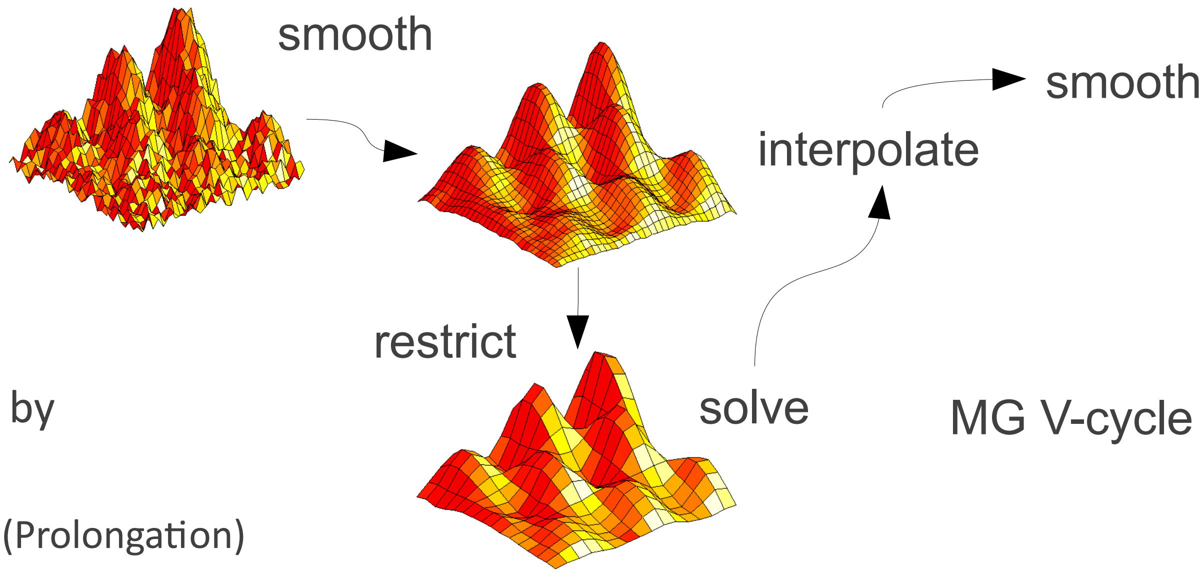
- Much of the work goes into solution
  - Typically over 50% for lattice generation
  - Can be over 90% for analysis

- Exhibits critical slowing down
  - Condition number diverges as mass decreases ($\kappa \sim 1/m$)
  - Standard Krylov solvers (CG, BiCGstab, …) become inefficient as condition number grows (iterations $\sim \sqrt{\kappa}$)

- Multigrid methods have been very successful in beating this in other fields

# Multigrid

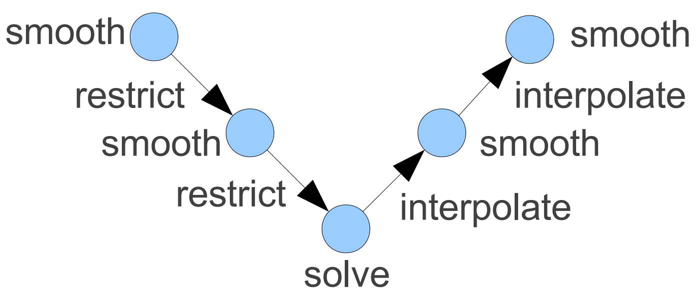
- Standard solvers (stationary, Krylov) good at reducing high frequency error components, not good with low frequency errors
- MG projects error onto coarse grid, solves, then interpolates correction back to fine grid

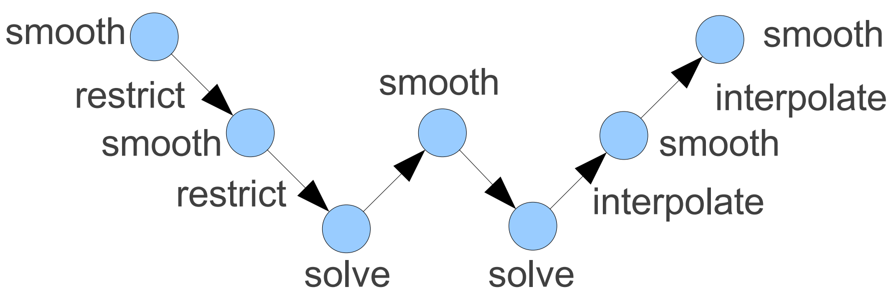



- V-cycle determined by
  - Restriction (R)
  - Interpolation (P) (Prolongation)
  - smoother

# Multigrid

- MG V-cycle typically used as preconditioner for outer solver
  - Here using GCR
- Used recursively: MG cycle used to solve on coarse grid, …
- Choice of cycle:
  - V-cycle, W-cycle, …
  - Here using GCR solver for coarse system with MG preconditioner



# Choosing R & P

- Coarse grid solve:

$$PA_c^{-1}Rr$$

$$A_c = RAP$$

- Algebraic MG: P & R formed from elements of A (or approximation to)
- Adaptive MG: P & R formed from slow-to-converge modes of A
  - Want P to preserve low modes of A
  - Form P from representative low modes chopped into blocks
  - R from low modes of A$^\dagger$

$$P = \begin{pmatrix} v1 & v2 & & & \\ v1 & v2 & & & \\ v1 & v2 & & & \\ & & v1 & v2 & \\ & & v1 & v2 & \\ & & v1 & v2 & \\ & & & & \ddots \end{pmatrix}$$

# Fine and coarse operators

- MG normally done on Hermitian positive definite systems ($D^\dagger D$)
  - Coarse operator constructed from Galerkin prescription $R = P^\dagger$, $A_c = P^\dagger A P$
  - Increases complexity of coarse operator (has 2-hop corner terms)
- Instead using just D
  - Want R to be rich in low left-modes
  - For $\gamma_5$-Hermitian operator can set $R = P^\dagger \gamma_5$
- Solving Wilson-clover operator
  - Using even-odd preconditioning on fine system
  - $D\,x = b \rightarrow D_p\,x_p = b \rightarrow D_r\,x_r = b_r$
  - Construct coarse operator from $D_p$ then construct reduced operator
  - $D_p$ no longer $\gamma_5$-Hermitian, but use same R anyway

$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix}$$

$$D_p = \begin{pmatrix} 1 & D_{eo} D_{oo}^{-1} \\ D_{oe} D_{ee}^{-1} & 1 \end{pmatrix}$$

$$D_r = 1 - D_{eo} D_{oo}^{-1} D_{oe} D_{ee}^{-1}$$

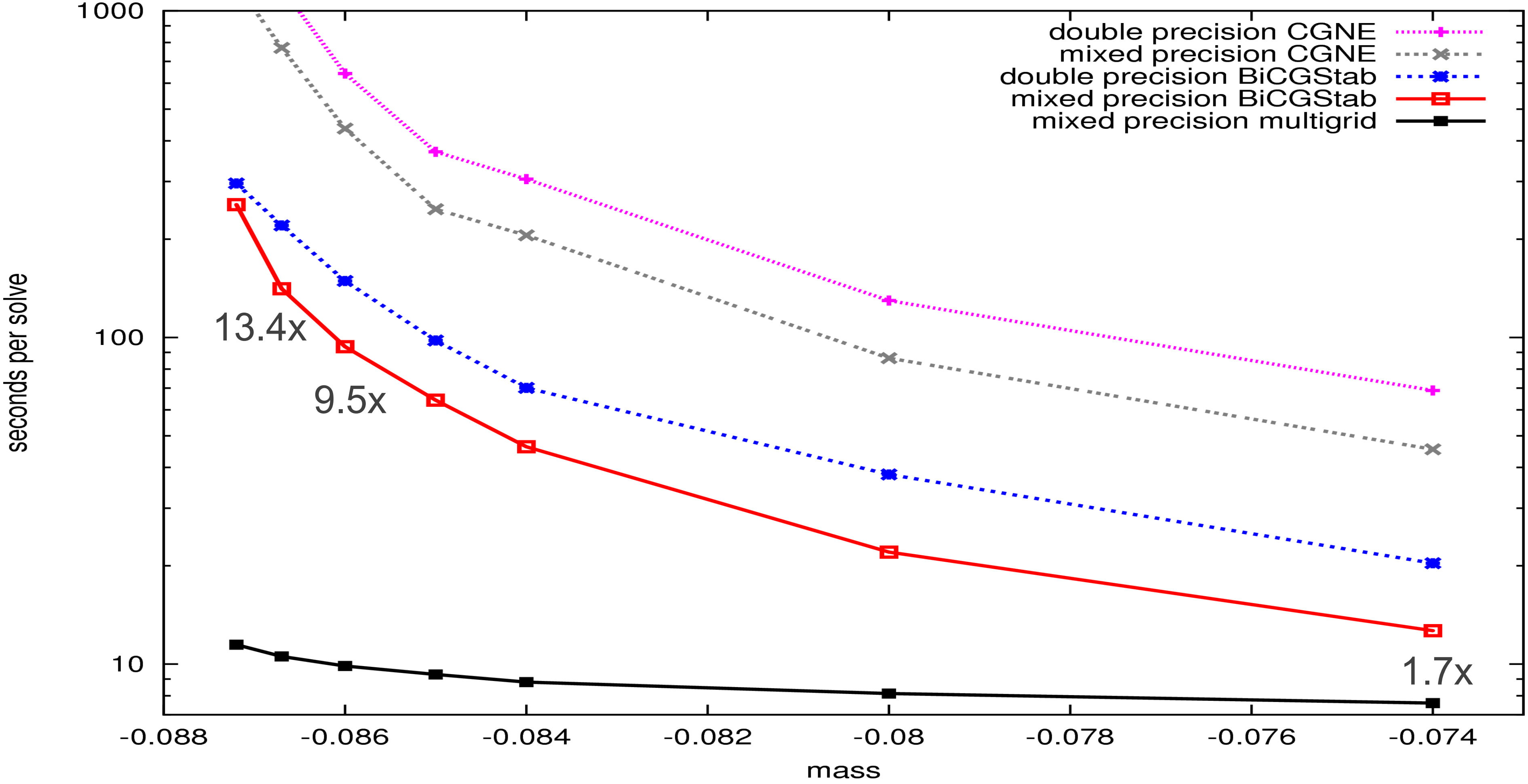
# Implementation Details

- Mixed precision
  - Outer GCR solver on fine level in double precision
  - MG preconditioner and all levels below in single
  - Comparison to mixed precision Krylov methods (iterative refinement)
- Implemented in US SciDAC QDP/C
  - Multi-lattice support and improved arbitrary Nc support

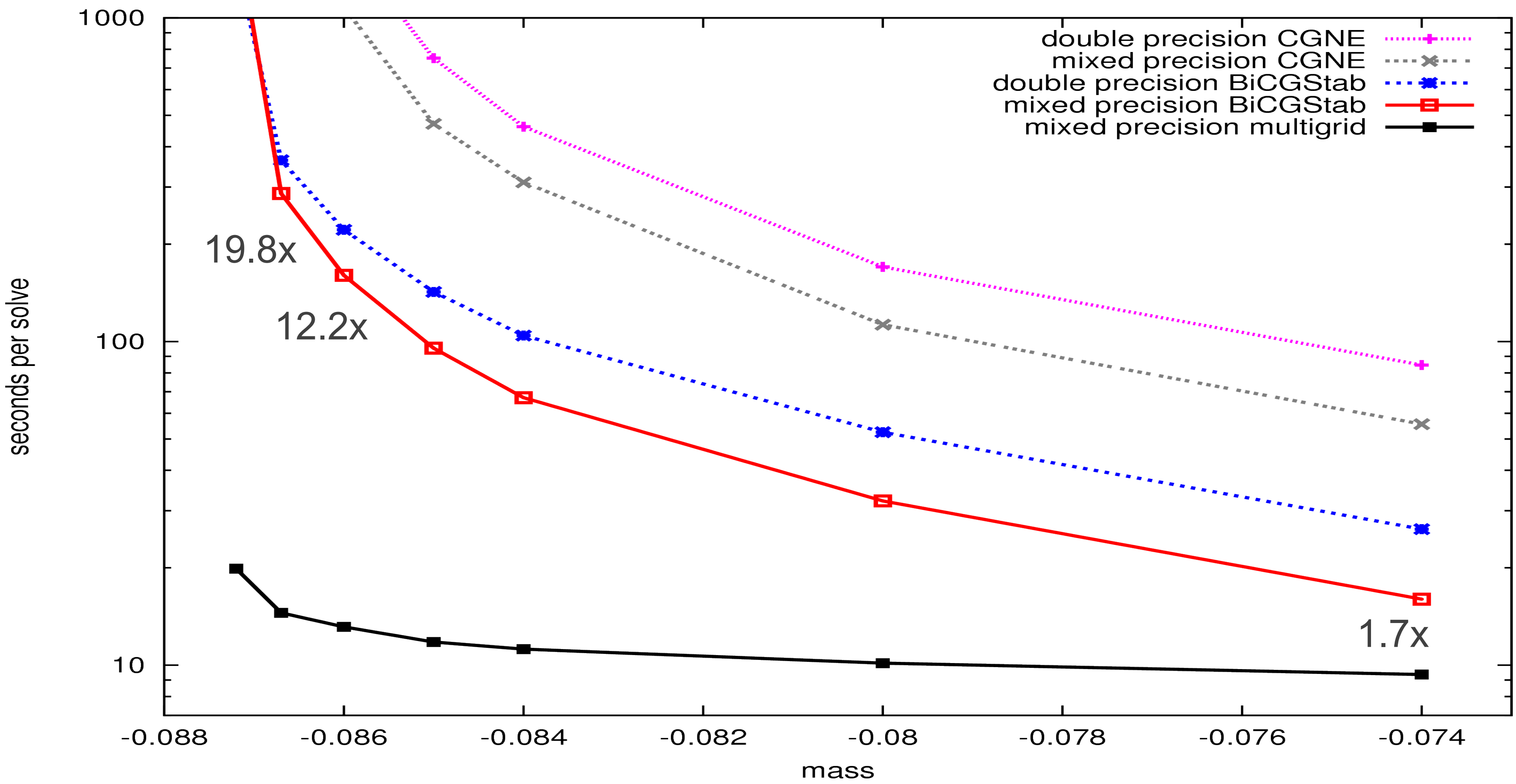
# Numerical results

- Using LHPC Hadron Spectrum Collaboration anisotropic clover lattices
  - $a_s \approx 3.5\ a_t$, $a_t \approx 0.1$ fm
  - $24^3$x128 and $32^3$x256
  - Dynamical $m_\pi \approx 220$ MeV (m = -0.086)
- Results obtained on BG/P
  - 256 cores for $24^3$x128
    - 1st coarse lattice: $8^3$x16 with 24 vectors
    - 2nd coarse lattice: $4^3$x4 with 32 vectors
  - 1024 cores for $32^3$x256
    - 1st coarse lattice: 16x8x8x32 with 24 vectors
    - 2nd coarse lattice: 4x4x4x16 with 32 vectors

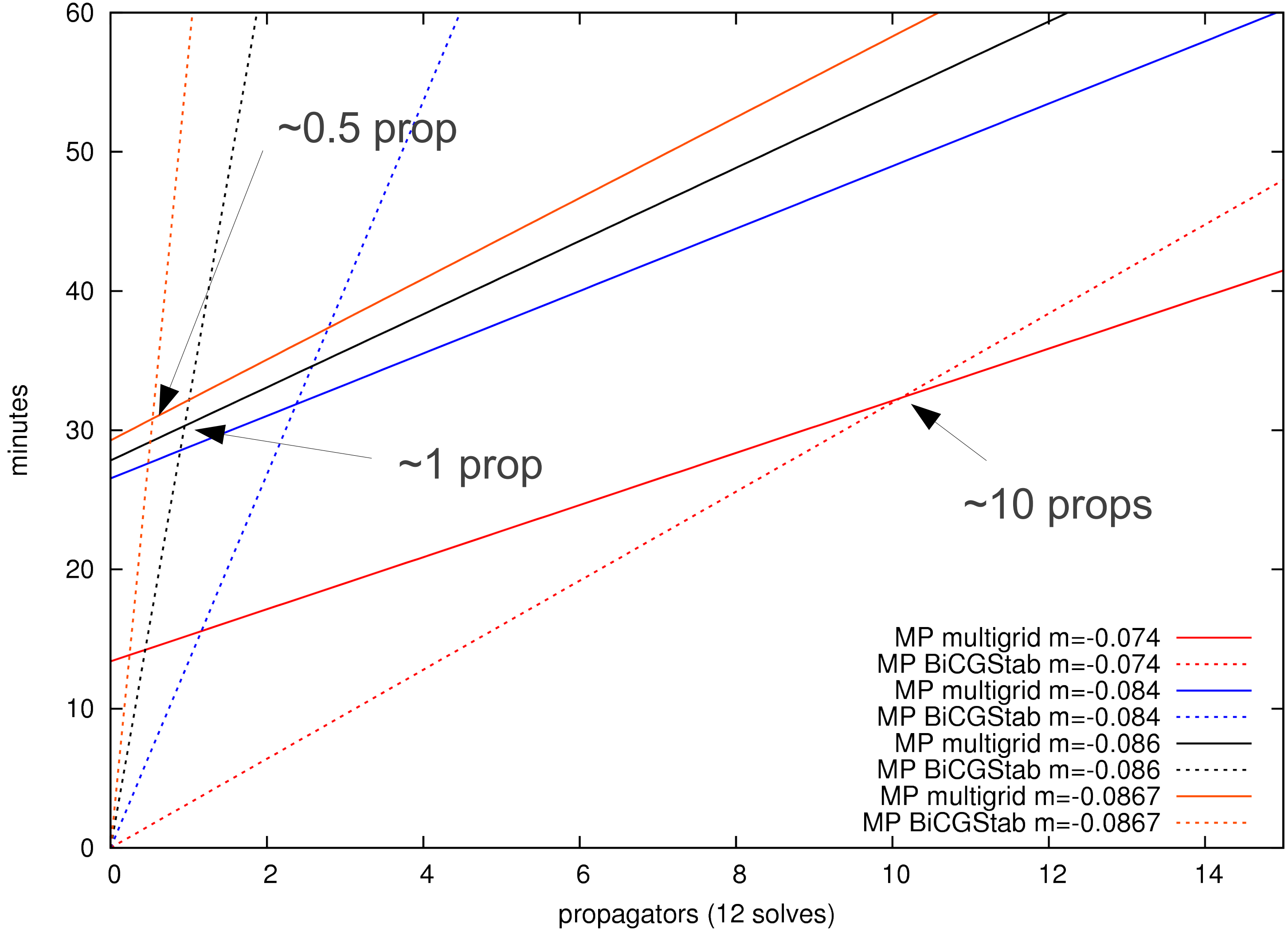
# Results $24^3$x128



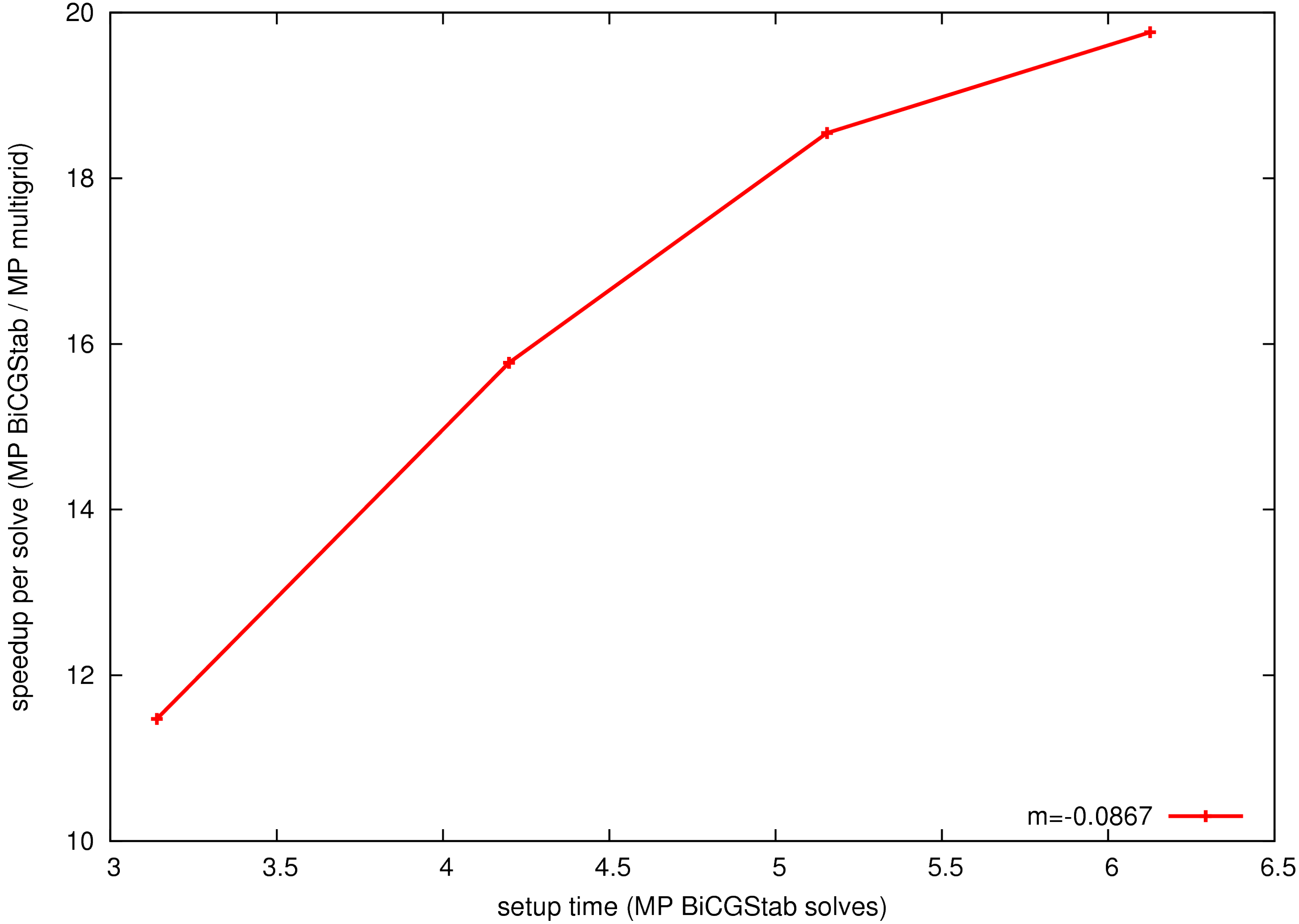
# Results $32^3$x256



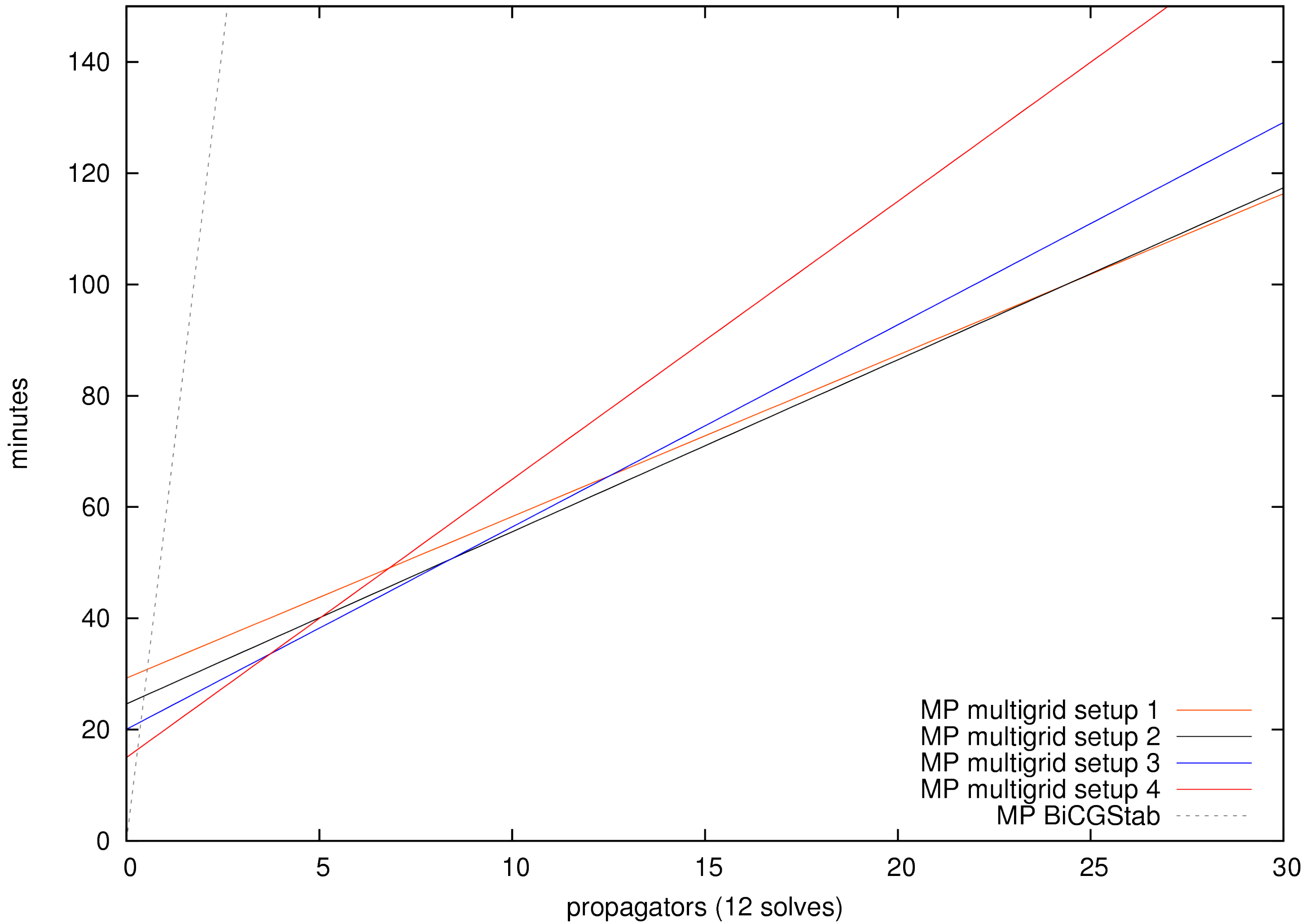
# Setup cost $32^3$x256



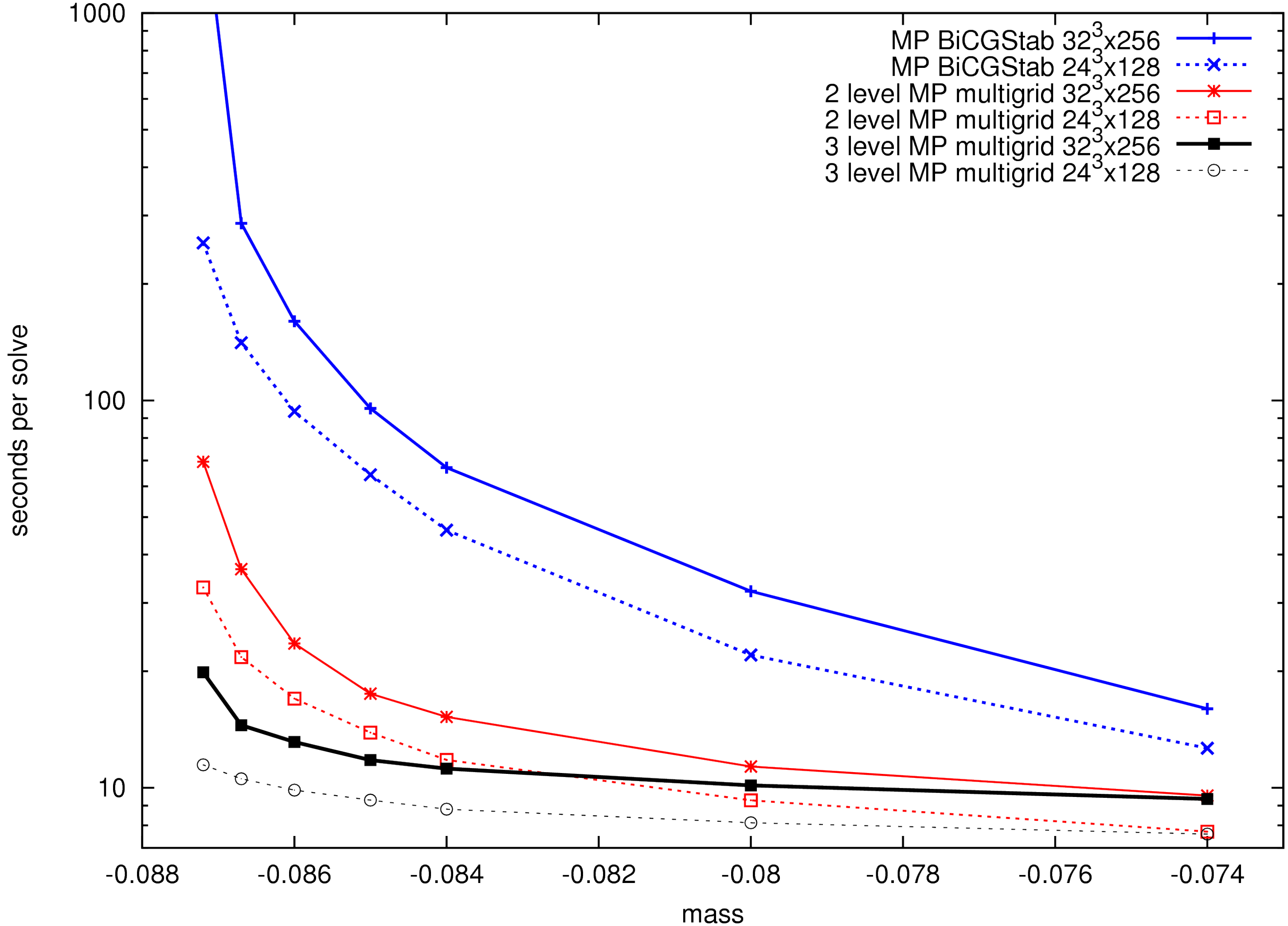
# Setup cost vs speedup $32^3$x256 (physical mass)



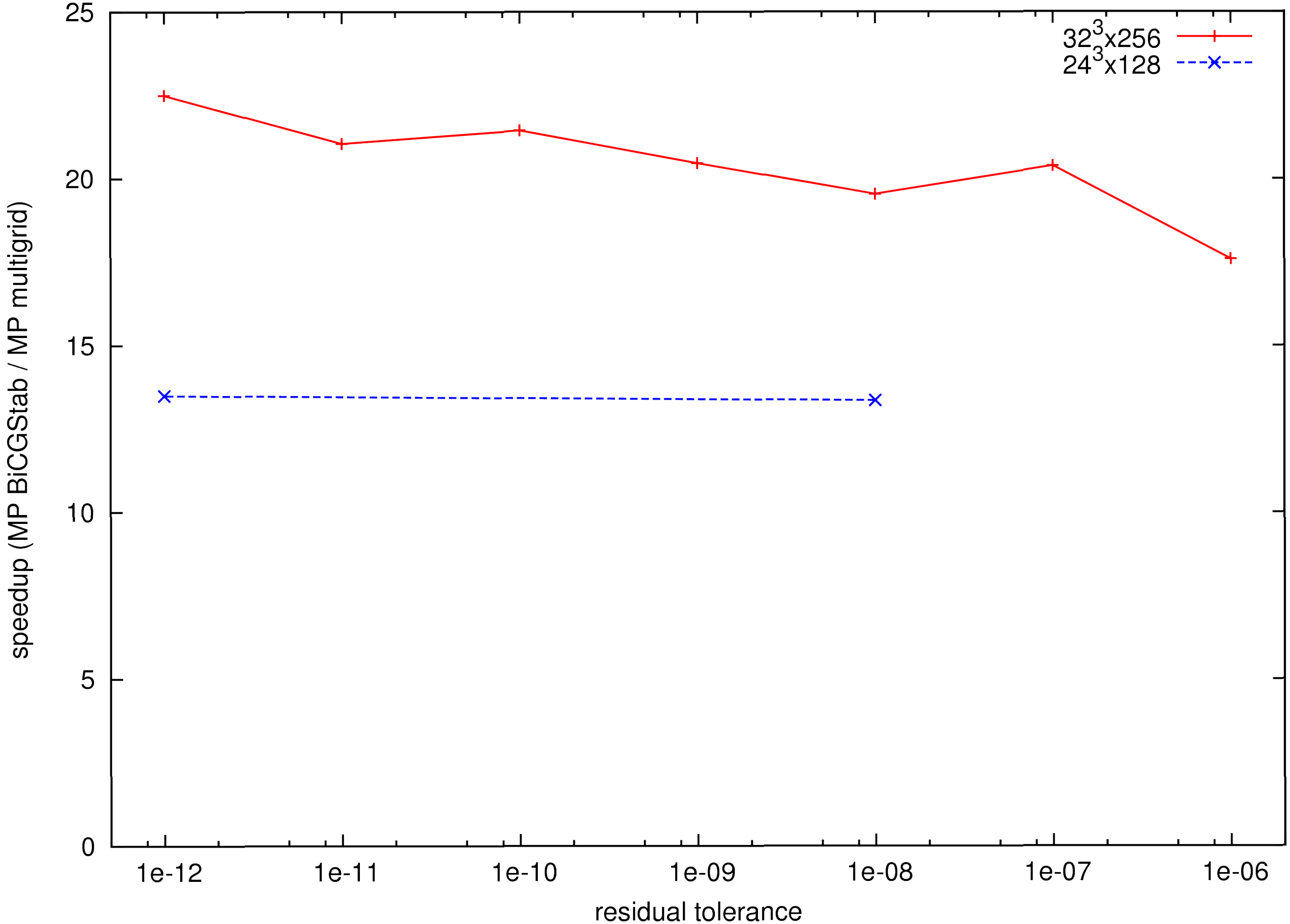
# $32^3$x256 setup cost



# 2 level vs 3 level



# Speedup vs residual



# Error vs residual

- Error:

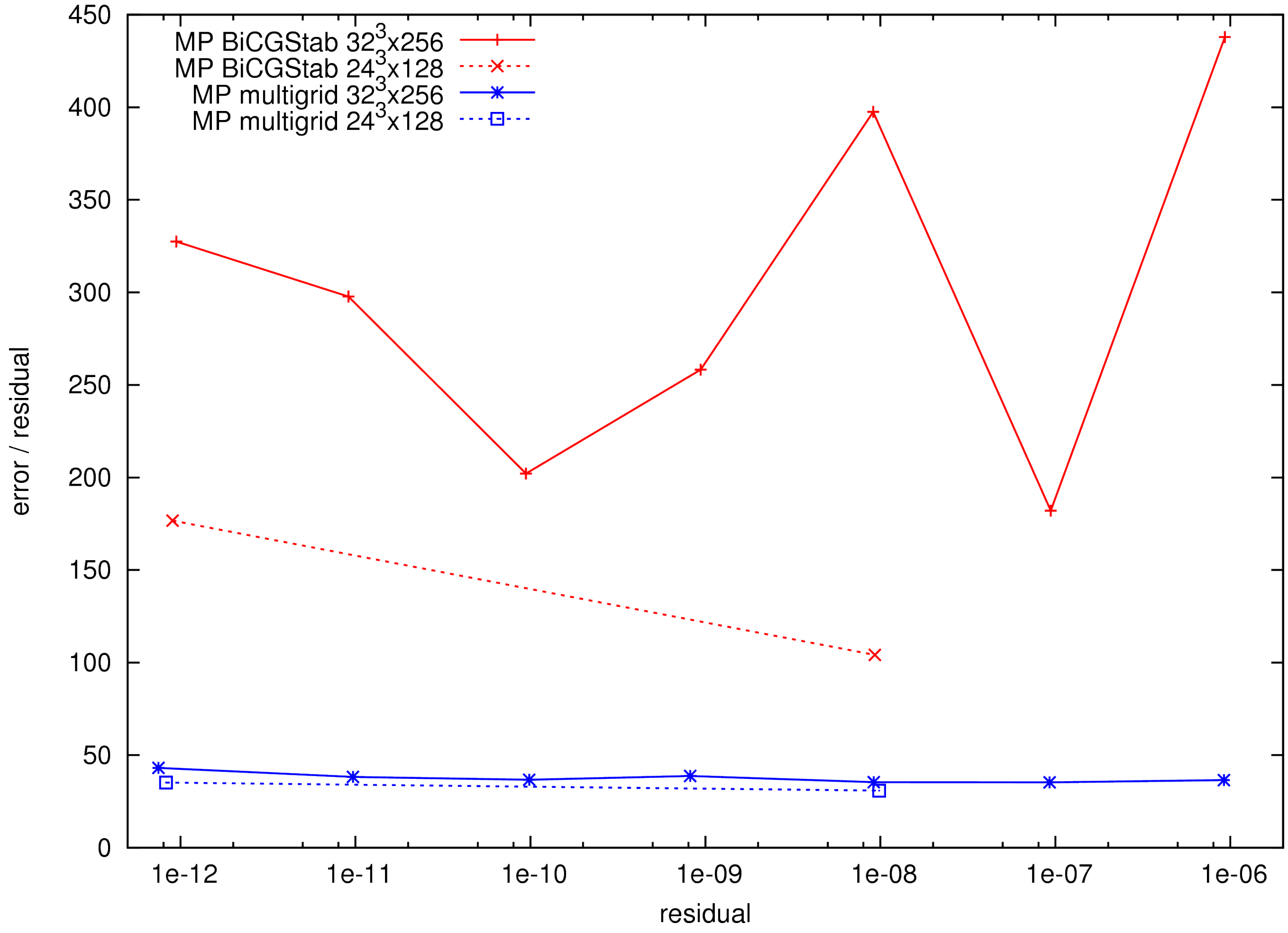
  $e = x^* - x$

- Residual:

  $r = b - A x$

  $= A e$

- Residual not as sensitive to low modes



# Setup methods

- Repeated Relaxation (inverse iteration) on random vectors
  - Simple (don't need to construct coarse operator)
  - Can vary number of iterations/cycles
  - Vectors may be locally redundant
- Adaptive smooth aggregation (αSA)
  - Construct new MG cycle with current vectors, use to find new vector
  - Requires construction of coarse operator
  - New vectors should be new important

# Summary and outlook

- Efficient implementation of Clover MG solver currently being used in production (disconnected diagrams)
- Gives 10-20x improvement for light quarks
- Error very stable and relatively small
- Speedup (and relative error) improves for larger lattices

- Test on larger lattices & extend to more levels
- Improve setup
  - Currently great for medium to large analysis projects
  - Extend to smaller projects and HMC
- Staggered & chiral quarks
- Port to GPUs