A Survey of Mixed Precision Multigrid Methods

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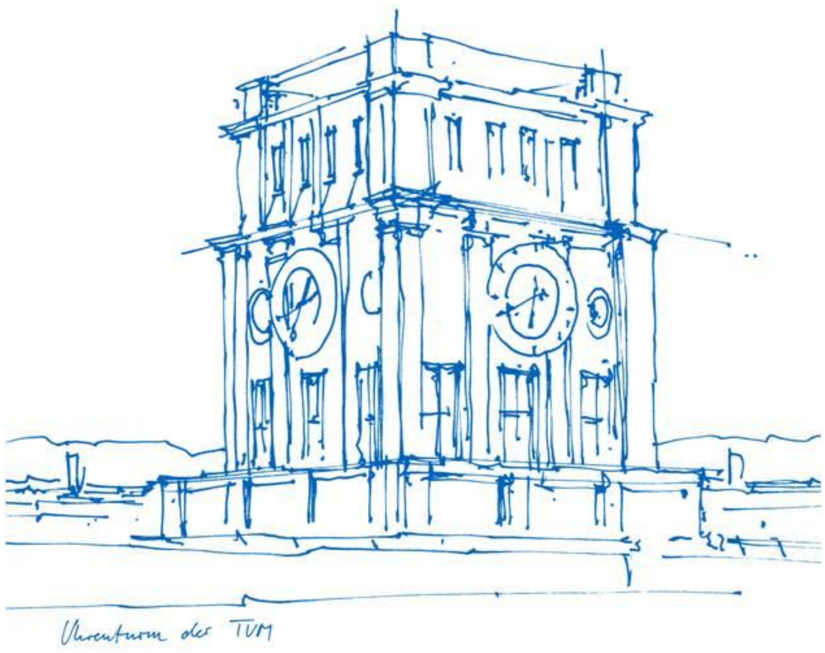


Content

Mixed Precision Algorithms

Motivation:

-> exponential growth of computational amount and increasing demand for speed
-> traditional high precision algorithms often become computationally prohibitive
-> balance between accuracy and computational efficientcy is needed

Definition:

Mixed precision algorithms: employ two or more precisions, selected from a limited set of available precisions (half, single, double by hardware and quadruple by software).

Multiprecision or variable precision algorithms: utilize one or more arbitrary precisions, which can vary based on the specific problem and are implemented through software.

Mixed Precision Algorithms

Accuracy:

- higher precision (represented by more bits) generally leads to higher accuracy
- computations involving extremely large or minuscule values, as well as those with subtle differences, will be more accurately captured.

Runtime:

- typically consists of data communication and computation
- data communication: a hardware-independent linear correlation with length of precision
- computational overhead: largely contingent upon the specific hardware architectures

Implementation:

Substitute high precision with low precision in the parts which are performance-sensitive but not error-sensitive.

Mixed Precision Algorithms

Physical simulations:

- PDE-based models: molecular dynamics simulation, computational fluid dynamics, computational electromagnetics
- most common and computationally intensive

Climate modelling and weather forecasting:

- inclination towards utilization of low precision since 2014
- low precision is sufficient to be consistent with observations on which a model is constructed

Machine learning:

- mixed precision training optimizer, such as the NVIDIA Apex library
- hardware accelerators that support mixed precision computations, such as NVIDIA's Tensor Cores

Multigrid Methods

- solve a linear system of equations (LSE) arising from PDEs
- compute across multiple grids of different resolutions
- **prolongation:** interpolate coarse grid to finer grid
- **restriction:** reduce fine grid to coarser grid
- **relaxation:** arbitrary LSE iterative solver

Multigrid Methods

Geometric multigrid methods:

- operate directly on a hierarchy of grids that are nested within each other
- further categorized: V-cycle, W-cycle, or Full Multigrid (FMG).

Algebraic multigrid methods:

- operate directly on the LSE derived from the discretization of the PDE
- construct a hierarchy of approximations based on the algebraic structure of the problem
- start with an initial approximation to the solution using coarse grid corrections

Multigrid Methods

Advantages:

- **Convergence**: exploit the multilevel structure to capture error components at different scales, leading to faster convergence rates
- **Scalability**: exhibit excellent scalability with problem size
- **Flexibility**: can be applied to structured, unstructured, and adaptive grids

Mixed precision algorithms:

- employ pure low precision multigrid methods as preconditioners for high precision solvers
- utilize different precisions at each level of the multigrid hierarchy

IEEE 754 Floating-Point Number Systems

Definition:

$$e \in \{e_{min}, \ldots, e_{max}\}$$

$$d_0, \ldots, d_{p-1} \in \{0, \ldots, b-1\}$$

$$x = \pm b^e \times \left(d_0 + \frac{d_1}{b} + \frac{d_2}{b^2} + \ldots + \frac{d_{p-1}}{b^{p-1}} \right)$$

Alternatively:

$$m \in \{0, b, \ldots, b^p - 1\}$$

$$x = \pm m \times b^{e-p+1}$$

Normalization:

$$d_0 \in \{1, \ldots, b-1\}$$

$$m \in \{b^{p-1}, b^{p-1} + b, \ldots, b^p - 1\}$$

Range:

$$b^{e_{min}} \leq |x| \leq b^{e_{max}} \times (b - b^{1-p})$$

IEEE 754 Floating-Point Number Systems

Format	Sign	Exponent	Significand	e_{min}	e_{max}	Machine Epsilon	x_{min}	x_{max}
FP16	1 bit	5 bits	10 bits	-14	+15	9.76×10^{-4}	6.10×10^{-5}	6.55×10^{4}
FP32	1 bit	8 bits	23 bits	-126	+127	1.19×10^{-7}	1.18×10^{-38}	3.40×10^{38}
FP64	1 bit	11 bits	52 bits	-1022	+1023	2.22×10^{-16}	2.22×10^{-308}	1.80×10^{308}
FP128	1 bit	15 bits	112 bits	-16382	+16383	1.93×10^{-34}	3.36×10^{-4932}	1.19×10^{4932}

Machine epsilon:

$$\epsilon = b^{1-p}$$

Unit roundoff:

$$u = \frac{1}{2} b^{1-p}$$

Subnormal numbers:

$$e = e^{e_{min}}$$
$$d_0 = 0$$
$$m \in \{0, b, ..., b^{p-1} - 1\}$$

Rounding Error Analysis Model

Floating-point estimates:

$$fl(x) = x(1+\delta), \ |\delta| \le u$$

Binary operations:

$$fl(x \star y) = (x \star y)(1+\delta), \ |\delta| \le u$$

Linear transformation:

$$fl(Ax) = Ax + \delta, \ |\delta| \le \frac{nu}{1-nu}|A| \cdot |x|$$

Residual calculation:

$$fl(Ax-b) = Ax - b + \delta, \ |\delta| \le \frac{(n+1)u}{1-(n+1)u}(|b| + |A| \cdot |x|)$$

$$\mathrm{fl}(Ax-b) = Ax - b + \delta, \quad |\delta| \le \varepsilon|Ax-b| + (1+\varepsilon)\frac{(n+1)\bar{\varepsilon}}{1-(n+1)\bar{\varepsilon}}(|b| + |A| \cdot |x|)$$

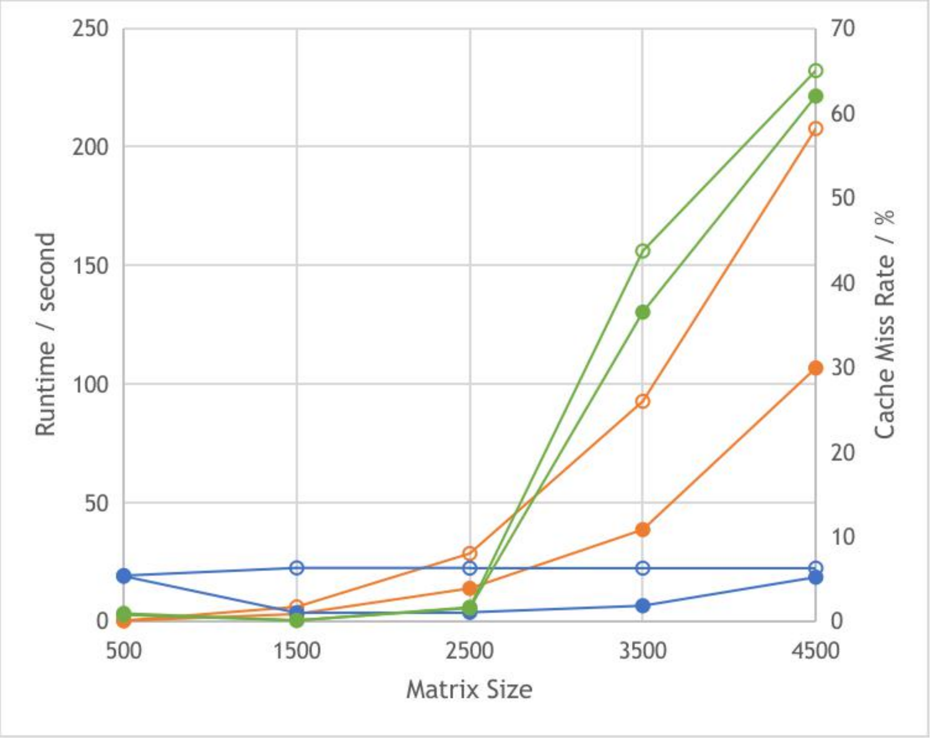
SuperMUC-NG

- Peak performance: 26.8 Peta FLOPS
- 9 islands, 6480 nodes
- 2 sockets per node
- 24 cores per socket (48 threads including hyperthreads per socket)
- Skylake EP: Intel Xeon 8174
- Frequencies:
  - Standard 2.7 GHz
  - Nominal 3.1 GHz
  - Peak 3.9 GHz
  - AVX 2.3 GHz
- Memory:
  - L1 instruction: 32KB
  - L1 data: 32KB
  - L2: 1MB
  - L3: 1.3MB / core, non-inclusive victim cache
  - DRAM: 96GB per node, aggregated bandwidth 128 GB / s

Matrix-Matrix Multiplication - Cache Optimization

```
for (int i = 0; i < n; i++) {
    for (int j = 0; j < n; j++) {
        for (int k = 0; k < n; k++) {
            C[i * n + j] += A[i * n + k] * B
                [k * n + j];
        }
    }
}
```

```
for (int i = 0; i < n; i++) {
    for (int k = 0; k < n; k++) {
        for (int j = 0; j < n; j++) {
            C[i * n + j] += A[i * n + k] * B
                [k * n + j];
        }
    }
}
```



orange: runtime
blue: L2 miss rate
green: L3 miss rate

empty symbols: original
filled symbols: optimized
single precision and -O1

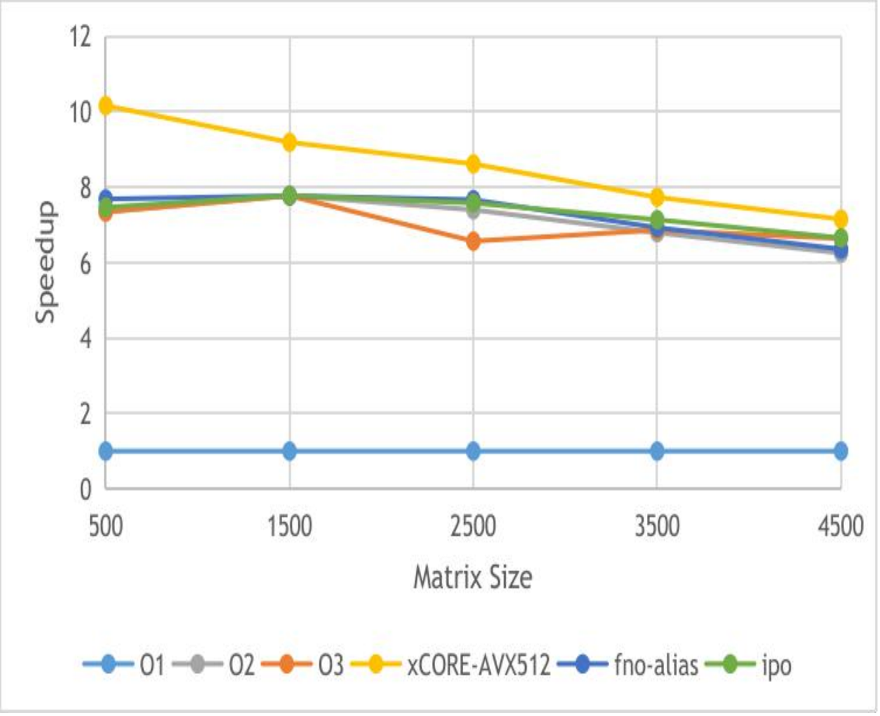
Matrix-Matrix Multiplication - Compiler Optimization

- -O1, -O2, and -O3: progressively enhanced optimization levels. The latter two enables SIMD vectorization. -O2 is used when no one is specified.

- -ipo: interprocedural optimization: perform optimization across different functions

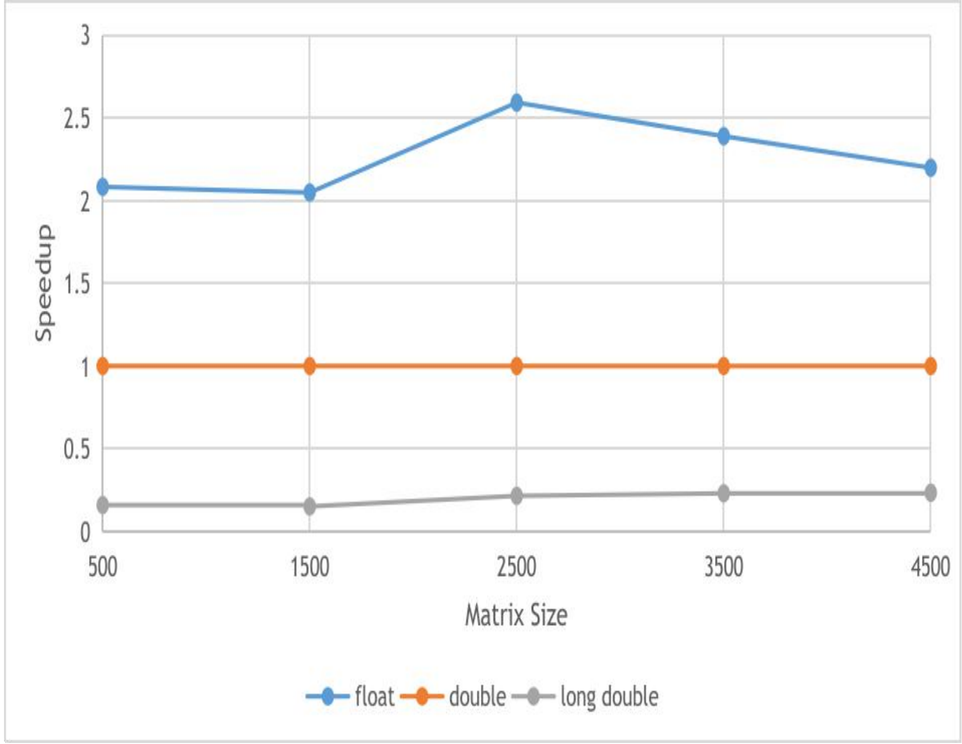
- -fno-alias: assume there is not memory aliasing and optimize further

- -xCORE-AVX512: utilizes broader vector registers and supplementary SIMD operations provided by the AVX-512 instruction set supported on SuperMUC-NG



single precision and optimized kernel

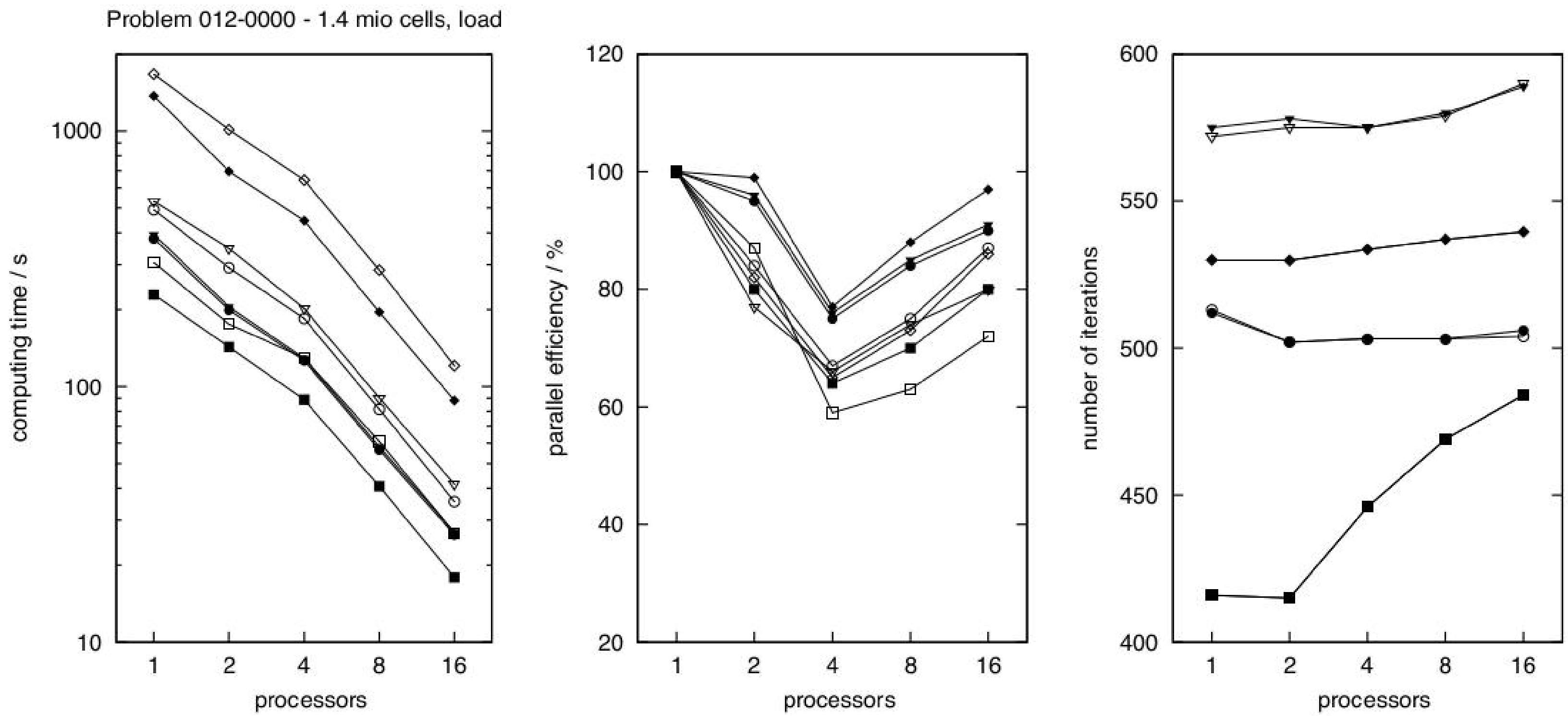
Matrix-Matrix Multiplication - Precision Optimization



optimized kernel and -O2

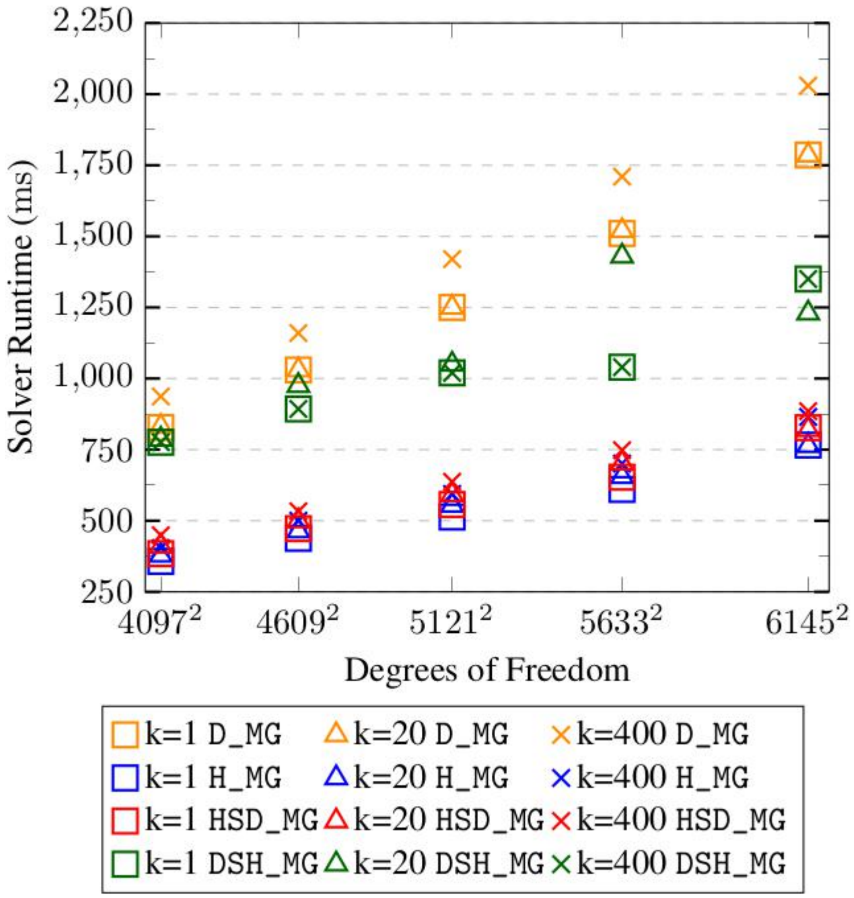
Performance Evaluation - CFD Simulation on CPU

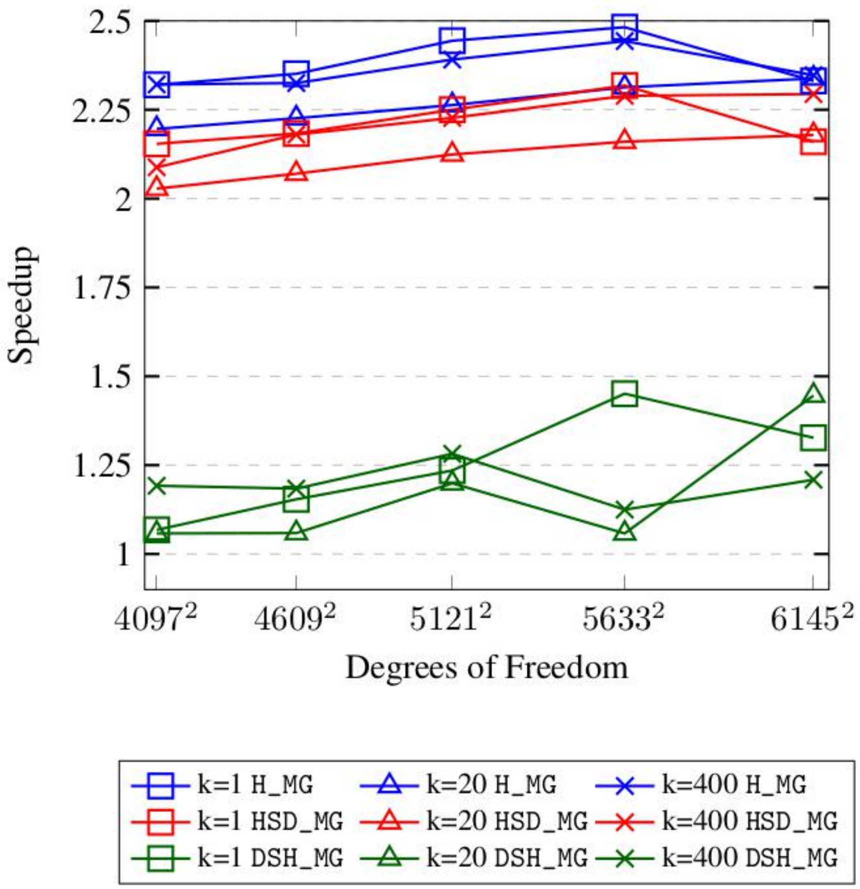
Double precision conjugate gradient algorithm preconditioned by **single** precision multigrid methods



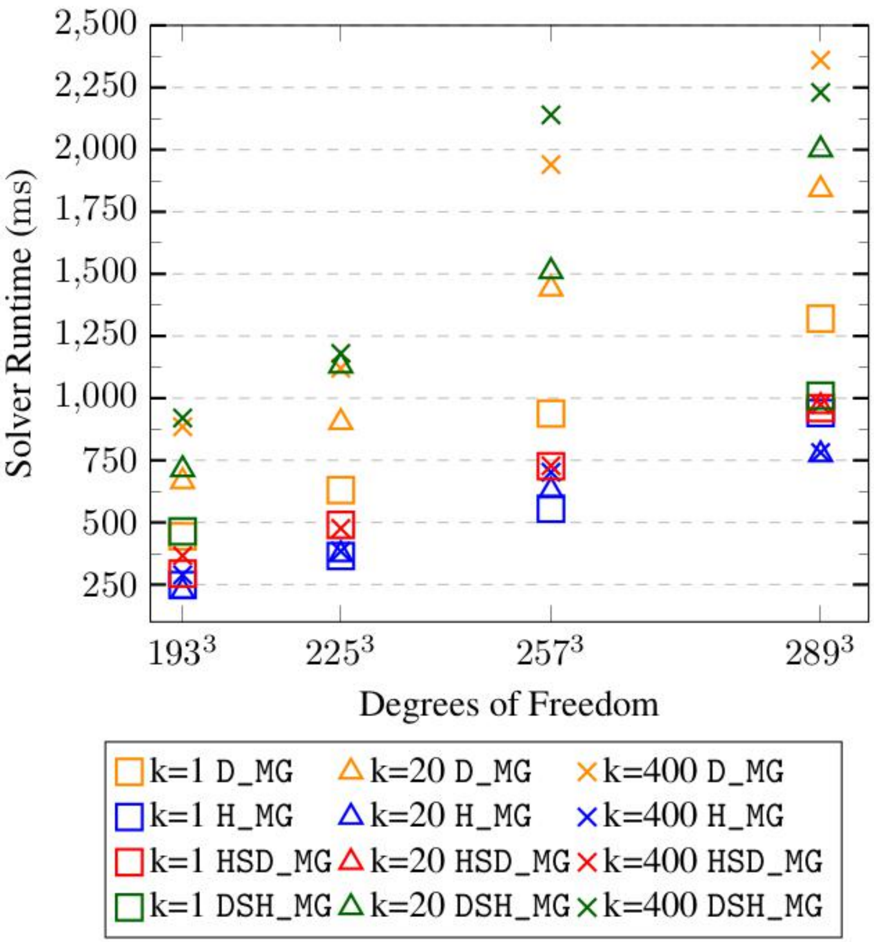
empty symbols: 8-bit; filled symbols: 4-bit; different markers mean different multigrid methods

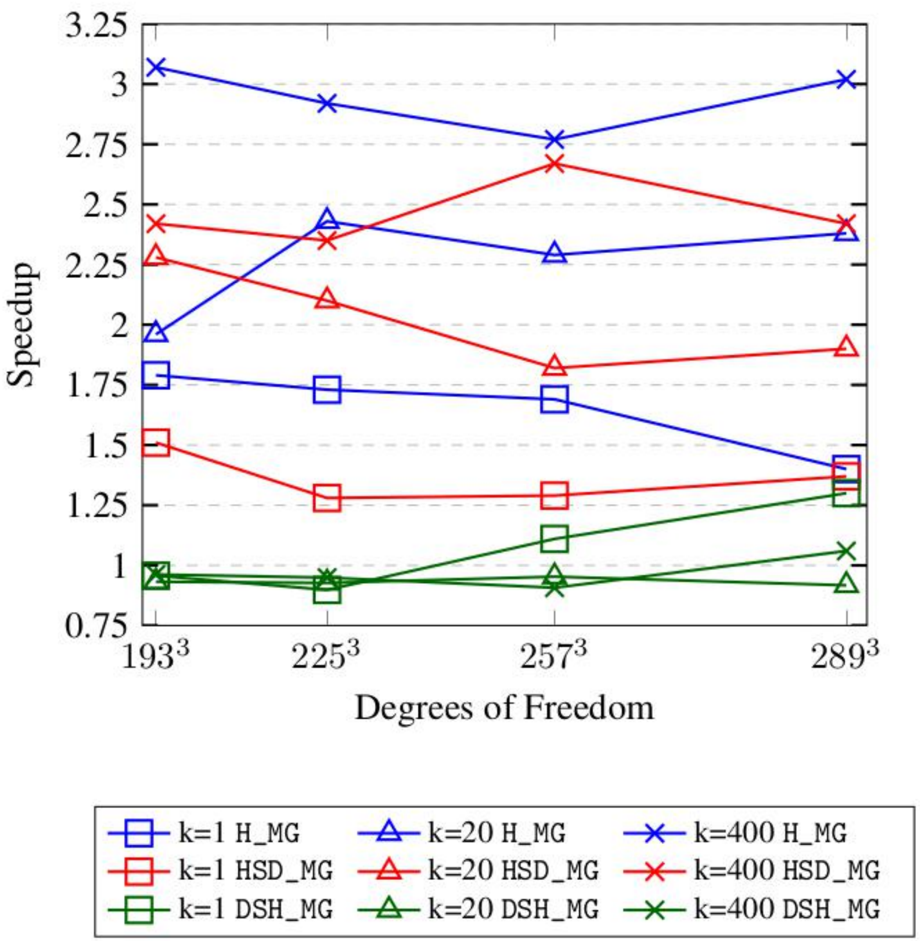
Performance Evaluation - 2D Poisson's Equation



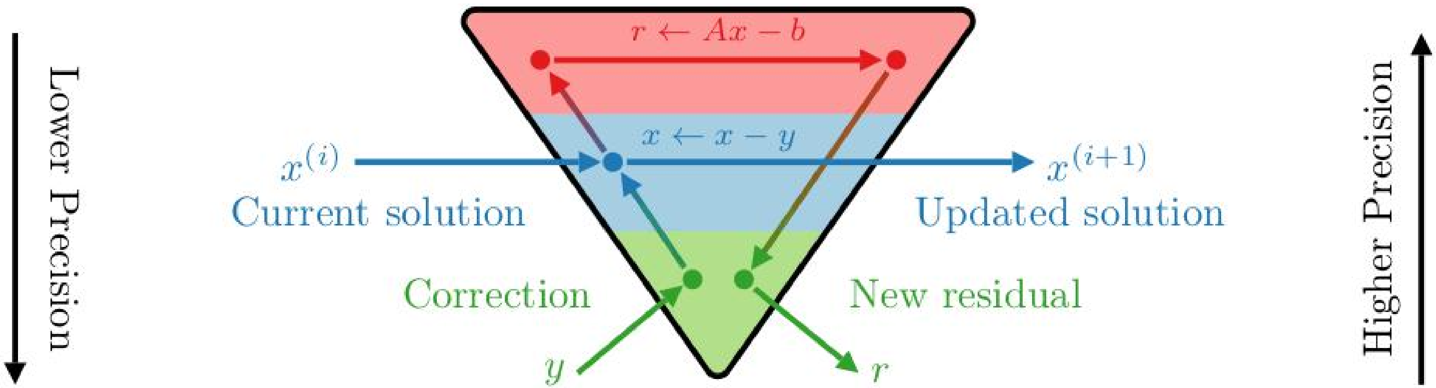


Performance Evaluation - 3D Poisson's Equation





Rounding Error Analysis - Iterative Refinement



Algorithm 3.1 `Iterative Refinement` ($\mathcal{IR}$)

Input: A, b, x initial guess, tol > 0 convergence tolerance.

1: $r \leftarrow Ax - b$ ▷ Compute $\mathcal{IR}$ Residual and Round
2: **if** $\|r\| <$ tol **then**
3:     **return** x ▷ Return Solution of $Ax = b$
4: **end if**
5: $y \leftarrow \mathtt{InnerSolve}(A, r)$ ▷ Compute Approximate Solution of $Ay = r$
6: $x \leftarrow x - y$ ▷ Update Approximate Solution of $Ax = b$
7: **goto** 1

Rounding Error Analysis - Iterative Refinement

Discrete energy norm:

$$\|x\|_A = \|A^{\frac{1}{2}}x\|, x \in \mathbb{R}^n$$

Condition numbers:

$$\kappa(A) = \|A\| \cdot \|A^{-1}\|$$

$$\underline{\kappa}(A) = \psi\|A^{-1}\|$$

$$\psi(A) = \||A|\|$$

Sparsity factor:

$$\bar{m}_A^+ = \frac{m_A + 1}{1 - (m_A + 1)\bar{\varepsilon}}$$

Bound-related parameters:

$$\dot{\tau} = \kappa^{\frac{1}{2}}\dot{\varepsilon}$$

$$\tau = \kappa^{\frac{1}{2}}\varepsilon$$

$$\bar{\tau} = \kappa\bar{\varepsilon}$$

$$\gamma = \frac{\kappa^{\frac{1}{2}} + \underline{\kappa}}{\kappa}$$

$$\bar{\varepsilon} \leq \varepsilon \leq \dot{\varepsilon}$$

Rounding Error Analysis - Iterative Refinement

Error bound of inner solver:

$$\|y - A^{-1}r\|_A \leq \rho\|A^{-1}r\|_A$$

Relative error bound:

$$\frac{\|x^{(i+1)} - A^{-1}b\|_A}{\|A^{-1}b\|_A} \leq \rho_{ir}\frac{\|x^{(i)} - A^{-1}b\|_A}{\|A^{-1}b\|_A} + \chi$$

Convergence factor:

$$\rho_{ir} = \rho + \delta_{\rho_{ir}}, \quad \delta_{\rho_{ir}} = \frac{(1+2\rho)\tau + \gamma(1+\rho)(1+\varepsilon)\bar{m}_A^+\bar{\tau}}{1-\tau}$$

Limiting accuracy:

$$\chi = \frac{\tau + \gamma(1+\rho)(1+\varepsilon)\bar{m}_A^+\bar{\tau}}{1-\tau}$$

Rounding Error Analysis - Iterative Refinement

Proof:

$$r = \underbrace{Ax^{(i)} - b}_{\text{exact residual}} + \underbrace{\delta_1}_{\varepsilon\text{-}\bar{\varepsilon}\text{ error}}, \quad |\delta_1| \leq \varepsilon|Ax^{(i)} - b| + (1+\varepsilon)\bar{m}_A^+\bar{\varepsilon}\left(|b| + |A|\cdot|x^{(i)}|\right)$$

$$\begin{aligned}
\left\|A^{-\frac{1}{2}}\left(|b| + |A|\cdot|x^{(i)}|\right)\right\| &\leq \|A^{-\frac{1}{2}}\|\left(\|AA^{-1}b\| + \psi\|x^{(i)}\|\right) \\
&\leq \|A^{-\frac{1}{2}}\|\cdot\|A^{\frac{1}{2}}\|\cdot\|A^{-1}b\|_A + \psi\|A^{-1}\|\cdot\|x^{(i)}\|_A \\
&= \kappa^{\frac{1}{2}}\|A^{-1}b\|_A + \underline{\kappa}\|x^{(i)}\|_A \\
&\leq (\kappa^{\frac{1}{2}} + \underline{\kappa})\|A^{-1}b\|_A + \underline{\kappa}\|x^{(i)} - A^{-1}b\|_A.
\end{aligned}$$

$$\begin{aligned}
\|A^{-1}\delta_1\|_A &= \|A^{-\frac{1}{2}}\delta_1\| \\
&\leq \varepsilon\|A^{-\frac{1}{2}}\|\cdot\|Ax^{(i)} - b\| + (1+\varepsilon)\bar{m}_A^+\bar{\varepsilon}\left\|A^{-\frac{1}{2}}\left(|b| + |A|\cdot|x^{(i)}|\right)\right\| \\
&\leq \varepsilon\kappa^{\frac{1}{2}}\|x^{(i)} - A^{-1}b\|_A \\
&\quad + (1+\varepsilon)\bar{m}_A^+\bar{\varepsilon}\left((\kappa^{\frac{1}{2}} + \underline{\kappa})\|A^{-1}b\|_A + \underline{\kappa}\|x^{(i)} - A^{-1}b\|_A\right).
\end{aligned}$$

Rounding Error Analysis - Iterative Refinement

$$
\begin{aligned}
&\|y - A^{-1}r\|_A \\
&\quad \le \rho\|A^{-1}r\|_A \\
&\quad = \rho\|A^{-1}\left(Ax^{(i)} - b + \delta_1\right)\|_A \\
&\quad \le \rho\left[\|x^{(i)} - A^{-1}b\|_A + \|A^{-1}\delta_1\|_A\right] \\
&\quad \le \rho\Big[(1+\varepsilon\kappa^{\frac{1}{2}})\|x^{(i)} - A^{-1}b\|_A \\
&\qquad + (1+\varepsilon)\bar{m}_A^{+}\bar{\varepsilon}\left((\kappa^{\frac{1}{2}} + \underline{\kappa})\|A^{-1}b\|_A + \underline{\kappa}\|x^{(i)} - A^{-1}b\|_A\right)\Big]
\end{aligned}
$$

$$
x^{(i+1)} = \underbrace{x^{(i)} - y}_{\text{exact update}} + \underbrace{\delta_2}_{\varepsilon \text{ error}}, \quad |\delta_2| \le \varepsilon|x^{(i+1)}|
$$

$$
\begin{aligned}
\|x^{(i+1)} - A^{-1}b\|_A &= \|x^{(i)} - A^{-1}b - A^{-1}r - (y - A^{-1}r) + \delta_2\|_A \\
&\le \|A^{-1}\delta_1 + (y - A^{-1}r)\|_A + \|\delta_2\|_A \\
&\le \|A^{-1}\delta_1\|_A + \|y - A^{-1}r\|_A + \varepsilon\|A^{\frac{1}{2}}\| \cdot \|x^{(i+1)}\| \\
&\le \left(\rho + (1+\rho)\varepsilon\kappa^{\frac{1}{2}})\right)\|x^{(i)} - A^{-1}b\|_A \\
&\quad + (1+\rho)(1+\varepsilon)\bar{m}_A^{+}\bar{\varepsilon}\left((\kappa^{\frac{1}{2}} + \underline{\kappa})\|A^{-1}b\|_A + \underline{\kappa}\|x^{(i)} - A^{-1}b\|_A\right) \\
&\quad + \varepsilon\kappa^{\frac{1}{2}}(\|x^{(i+1)} - A^{-1}b\|_A + \|A^{-1}b\|_A) \\
&= \varepsilon\kappa^{\frac{1}{2}}\|x^{(i+1)} - A^{-1}b\|_A + (\rho + \delta_3)\|x^{(i)} - A^{-1}b\|_A \\
&\quad + \left(\varepsilon\kappa^{\frac{1}{2}} + (1+\rho)(1+\varepsilon)\bar{m}_A^{+}\bar{\varepsilon}(\kappa^{\frac{1}{2}} + \underline{\kappa})\right)\|A^{-1}b\|_A,
\end{aligned}
$$

$$
\delta_3 = (1+\rho)\left(\varepsilon\kappa^{\frac{1}{2}} + (1+\varepsilon)\bar{m}_A^{+}\bar{\varepsilon}\underline{\kappa}\right)
$$

$$
\frac{\rho + \delta_3}{1 - \varepsilon\kappa^{\frac{1}{2}}} = \rho + \frac{\delta_3 + \rho\varepsilon\kappa^{\frac{1}{2}}}{1 - \varepsilon\kappa^{\frac{1}{2}}} = \rho + \delta_{\rho_{ir}}
$$

$$
\sum_{i=0}^{N-1}(\rho + \delta_{\rho_{ir}})^i \le \frac{1}{1 - (\rho + \delta_{\rho_{ir}})}
$$

$\square$

Rounding Error Analysis - Two Grid

Algorithm 5.1 `Two-Grid (`$\mathcal{TG}$`) Correction Scheme`

Input: A, r, P, M.

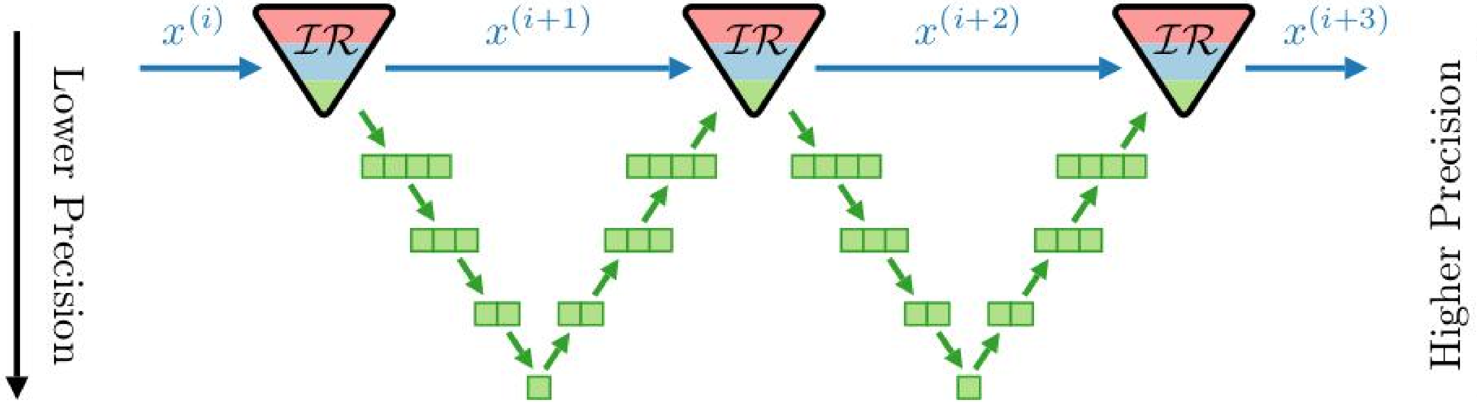
$r \leftarrow r$ ▷ Round RHS and Initialize $\mathcal{TG}$
$y \leftarrow Mr$ ▷ Relax on Current Approximation ($y = 0$)
$r_{\mathrm{tg}} \leftarrow Ay - r$ ▷ Evaluate $\mathcal{TG}$ Residual
$b_c \leftarrow P^t r_{\mathrm{tg}}$ ▷ Restrict $\mathcal{TG}$ Residual to Coarse-Level
$d_c \leftarrow B_c(P^t AP)^{-1} b_c$ ▷ Solve Coarse-Level Equation
$d \leftarrow Pd_c$ ▷ Interpolate Correction to Fine Level
$y \leftarrow y - d$ ▷ Update Approximate Solution of $Ay = r$
return y ▷ Return Approximate Solution of $Ay = r$

Convergence established:

$$\|y - A^{-1}r\|_A \leq \rho_{tg}\|A^{-1}r\|_A, \quad \rho_{tg} = \rho_{tg}^* + \delta_{\rho_{tg}}$$

$$\delta_{\rho_{tg}} = \delta_{\rho_{tg}}(\dot{\tau}) = a_1\dot{\tau} + a_2\dot{\tau}^2 + a_3\dot{\tau}^3$$

Rounding Error Analysis - V(1,0)-Cycle

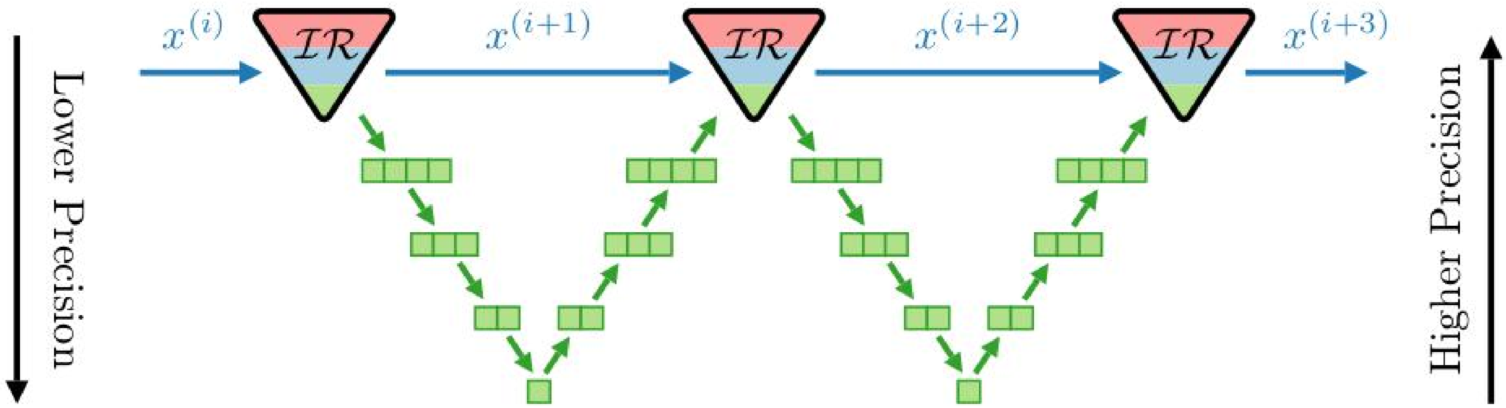


Algorithm 6.1 `V(1,0)-Cycle (`$\mathcal{V}$`) Correction Scheme`

Input: A, r, P, $\ell \geq 1$ $\mathcal{V}$ levels.

$r \leftarrow r$ ▷ Round RHS and Initialize $\mathcal{V}$
$y \leftarrow Mr$ ▷ Relax on Current Approximation ($y = 0$)
if $\ell > 1$ **then** ▷ Check for Coarser Level
  $r_{\mathrm{V}} \leftarrow Ay - r$ ▷ Evaluate $\mathcal{V}$ Residual
  $r_{\ell-1} \leftarrow P^t r_{\mathrm{V}}$ ▷ Restrict $\mathcal{V}$ Residual to Coarse-Level
  $d_{\ell-1} \leftarrow \mathcal{V}(A_{\ell-1}, r_{\ell-1}, P_{\ell-1}, \ell - 1)$ ▷ Compute Correction from Coarser Levels
  $d \leftarrow P d_{\ell-1}$ ▷ Interpolate Correction to Fine Level
  $y \leftarrow y - d$ ▷ Update Approximate Solution of $Ay = r$
end if
return y ▷ Return Approximate Solution of $Ay = r$

Rounding Error Analysis - V(1,0)-Cycle



Precision coarsening factor:

$$\dot{\zeta}_j = \frac{\dot{\varepsilon}_{j-1}}{\dot{\varepsilon}_j}, 2 \leq j \leq \ell$$

Pseudo mesh-refinement factor:

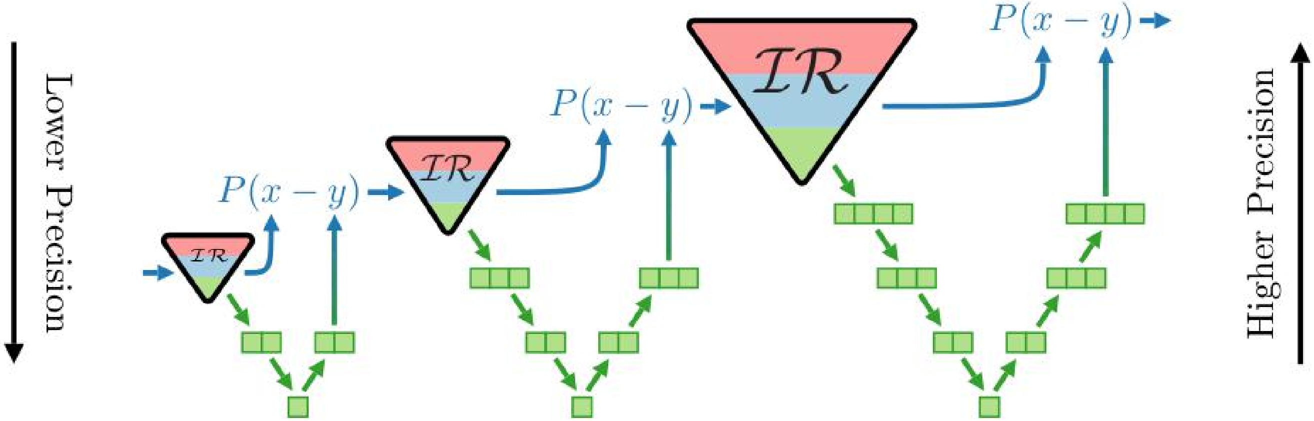
$$\theta_j = \frac{h_{j-1}}{h_j}, \quad 2 \leq j \leq \ell$$

Convergence established:

$$\|y - A^{-1}r\|_A \leq \rho_v \|A^{-1}r\|_A, \; \rho_v = \rho_v^* + \delta_{\rho_v}, \; \delta_{\rho_v} = \delta_{\rho_v}(\dot{\tau}_\ell) = \frac{\vartheta^m}{\vartheta^m - 1}\delta_{\rho_{tg}}(\dot{\tau}_\ell) \;,$$

where $\vartheta = \min_{1 \leq j \leq \ell} \{\theta_j \dot{\zeta}_j^{-\frac{1}{m}}\}$

Rounding Error Analysis - Full Multigrid

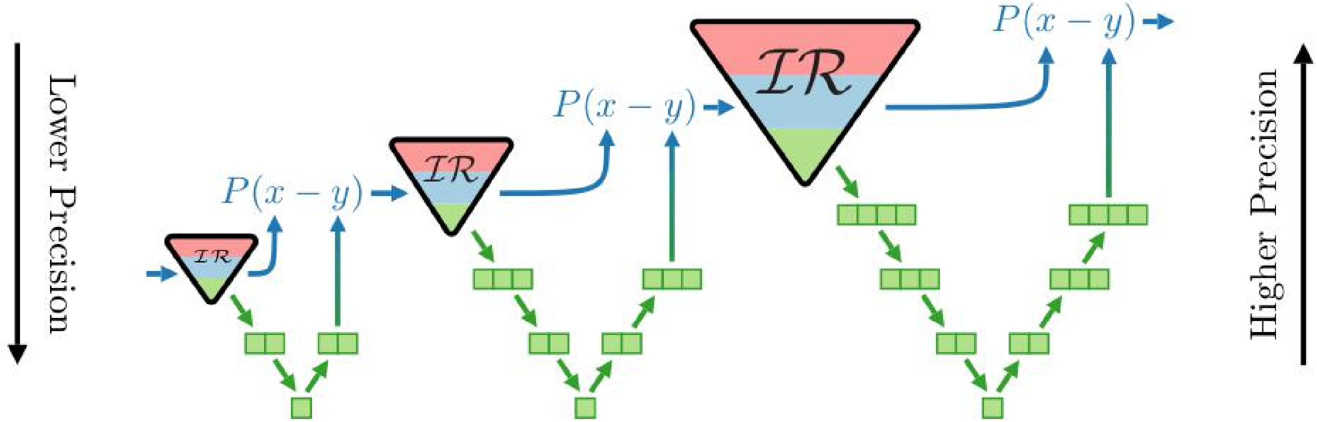


Algorithm 9.1 $\texttt{FMG}(1,0)\texttt{-Cycle}$ $(\mathcal{FMG})$

Input: A, b, P, $N \geq 1$ $\mathcal{IR}$ cycles (using one V$(1,0)$ each), $\ell \geq 1$ $\mathcal{FMG}$ levels.

$x \leftarrow 0$ ▷ Initialize $\mathcal{FMG}$
if $\ell > 1$ **then** ▷ Check for Coarser Level
  $x_{\ell-1} \leftarrow \mathcal{FMG}(A_{\ell-1}, b_{\ell-1}, P_{\ell-1}, \ell-1, N)$ ▷ Compute Coarse-Level Approximation
  $x \leftarrow P x_{\ell-1}$ ▷ Interpolate Approximation to Fine Level
end if
$i \leftarrow 0$ ▷ Initialize $\mathcal{IR}$
while $i < N$ **do**
  $r \leftarrow Ax - b$ ▷ Update $\mathcal{IR}$ Residual and Round
  $y \leftarrow \mathcal{V}(A, r, P, \ell)$ ▷ Compute Correction by $\mathcal{V}$
  $i \leftarrow i + 1$ ▷ Increment $\mathcal{IR}$ Cycle Counter
  $x \leftarrow x - y$ ▷ Update Approximate Solution of $Ax = b$
end while
return x ▷ Return Approximate Solution of $Ax = b$

Rounding Error Analysis - Full Multigrid



Assume:

$\rho_v + \delta_{\rho_{ir}} < 1$

χ is small enough

N is large enough

Then:

$$(\rho_v + \delta_{\rho_{ir}})^N \left((\sqrt{2} + \mu\tau)\theta^q C h^q + \mu\tau \right) + \frac{\chi}{1 - (\rho_v + \delta_{\rho_{ir}})} \leq C h^q$$ holds on all levels j.

Here $\mu = \mu_j = \kappa^{\frac{1}{2}}(P_j^t P_j) m_P^+$, h is pseudo mesh size, C and q are positive constants.

References

Main references for the presentation:

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The full list is presented in my paper.

THANKS