Using artificial intelligence and transprecision computing for accelerating earthquake simulation on Summit

Kohei Fujita and Takuma Yamaguchi
Earthquake Research Institute & Department of Civil Engineering, The University of Tokyo
Introduction

• Further speedup of physics-based simulation required for solving complex problems in seismology & earthquake engineering
  • Development of new methods required to get best performance on large-scale supercomputer systems such as Summit

• In this talk, we review our work on accelerating finite-element earthquake simulation on Summit using artificial intelligence and transprecision computing methods
  • Nominated for Gordon Bell Prize Finalist in SC18

A Fast Scalable Implicit Solver for Nonlinear Time-Evolution Earthquake City Problem on Low-Ordered Unstructured Finite Elements with Artificial Intelligence and Transprecision Computing

Tsuyoshi Ichimura\textsuperscript{1,2,3}, Kohei Fujita\textsuperscript{1,3}, Takuma Yamaguchi\textsuperscript{1}, Akira Naruse\textsuperscript{4}, Jack C. Wells\textsuperscript{5}, Thomas C. Schulthess\textsuperscript{6}, Tjerk P. Straatsma\textsuperscript{5}, Christopher J. Zimmer\textsuperscript{5}, Maxime Martinasso\textsuperscript{6}, Kengo Nakajima\textsuperscript{7,3}, Muneo Hori\textsuperscript{1,3}, Lalith Maddegrada\textsuperscript{1,3}

\textsuperscript{1}Earthquake Research Institute & Department of Civil Engineering, The University of Tokyo
\textsuperscript{2}Center for Advanced Intelligence Project, RIKEN
\textsuperscript{3}Center for Computational Science, RIKEN
\textsuperscript{4}NVIDIA Corporation, \textsuperscript{5}Oak Ridge National Laboratory
\textsuperscript{6}Swiss National Supercomputing Centre, \textsuperscript{7}Information Technology Center, The University of Tokyo
Smart cities

- Controlling cities based on real-time data for higher efficiency
- Computer modeling via high-performance computing is expected as key enabling tool
- Disaster resiliency is requirement; however, not established yet

Example of highly dense city: Tokyo Station district
Fully coupled aboveground/underground earthquake simulation required for resilient smart city
Earthquake modeling of smart cities

• Unstructured mesh with implicit solvers required for urban earthquake modeling
  • We have been developing high-performance implicit unstructured finite-element solvers (SC14 & SC15 Gordon Bell Prize Finalist, SC16 best poster)
• However, simulation for smart cities requires full coupling in super-fine resolution
  • Traditional physics-based modeling too costly
  • Can we combine use of data analytics to solve this problem?

SC14, SC15 & SC16 solvers: ground simulation only

Fully coupled ground-structure simulation with underground structures
Data analytics and equation based modeling

- Equation based modeling
  - Highly precise, but costly
- Data analytics
  - Fast inferencing, but accuracy not as high
- Use both methods to complement each other
Integration of data analytics and equation based modeling

• First step: use data generated by equation based modeling for data analytics training
  • Use high-performance computing in equation based modeling to generate very large amounts of high quality data
  • We developed earthquake intensity prediction method using this approach (SC17 Best Poster)

SC17

Phenomena

Data analytics (with better prediction)

Simulated data for training

Equation based modeling

• SC14: equation based modeling
• SC15: equation based modeling
• SC16: equation based modeling
• SC17: equation based modeling for AI
Integration of data analytics and equation based modeling

• We extend this concept in this paper: train AI to accelerate
  equation based modeling

SC18

Phenomena

Data analytics

AI for accelerating equation based solver

Equation based modeling (25-fold speedup from without AI)

• SC14: equation based modeling
• SC15: equation based modeling
• SC16: equation based modeling
• SC17: equation based modeling for AI
• SC18: AI for equation based modeling
Earthquake modeling for smart cities

- By using AI-enhanced solver, we enabled fully coupled ground-structure simulation on Summit.
Algorithm design of AI-enhanced solver
Difficulties of using data analytics to accelerate equation based modeling

- Target: Solve $A x = f$
- Difficulty in using data analytics in solver
  - Data analytics results are not always accurate
  - We need to design solver algorithm that enables robust and cost effective use of data analytics, together with uniformity for scalability on large-scale systems
- Candidates: Guess $A^{-1}$ for use in preconditioner
  - For example, we can use data analytics to determine the fill-in of matrix; however, challenging for unstructured mesh where sparseness of matrix $A$ is nonuniform (difficult for load balancing and robustness)
    - Manipulation of $A$ without additional information may be difficult…
Designing solver suitable for use with AI

• Use information of underlying governing equation
  • Governing equation’s characteristics with discretization conditions should include information about the difficulty of convergence in solver
  • Extract parts with bad convergence using AI and extensively solve extracted part
Solver suitable for use with AI

- Transform solver such that AI can be used robustly
  - Select part of domain to be extensively solved in adaptive conjugate gradient solver
  - Based on the governing equation’s properties, part of problem with bad convergence is selected using AI

\[
\text{PreCG}^c (1^{\text{st}} \text{ order tetrahedral mesh}) \quad \text{PreCG}^c_{\text{part}} (1^{\text{st}} \text{ order tetrahedral mesh}) \quad \text{PreCG} (2^{\text{nd}} \text{ order tetrahedral mesh})
\]

- Use \( z^c \) as initial solution
- Use \( z^c_{\text{cp}} \) as initial solution
- Use \( z \) for search direction

\[
\text{Approximately solve } A^c z^c = r^c \quad \text{Approximately solve } A^c_{\text{cp}} z^c_{\text{cp}} = r^c_{\text{cp}} \quad \text{Approximately solve } A z = r
\]

Loop until converged
How to select part of problem using AI

• In discretized form, governing equation becomes function of material property, element and node connectivity and coordinates
  • Train an Artificial Neural Network (ANN) to guess the degree of difficulty of convergence from these data

Whole city model

Extracted part by AI (about 1/10 of whole model)
Example of part selection using AI

- About 1/10 of domain is selected using generated ANN
  - Cost per iteration of selective solving is 1/10 of standard solver
Performance of solver with AI

- FLOP count decreased by 5.56-times from PCGE (standard solver; Conjugate Gradient solver with block Jacobi preconditioning)

<table>
<thead>
<tr>
<th></th>
<th>Without AI</th>
<th>With AI</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG iterations</td>
<td>132,665</td>
<td>88</td>
</tr>
<tr>
<td>$PreCG^c$ iterations</td>
<td>-</td>
<td>5,803</td>
</tr>
<tr>
<td>$PreCG^c_{part}$ iterations</td>
<td>-</td>
<td>26,826</td>
</tr>
<tr>
<td>$PreCG$ iterations</td>
<td>-</td>
<td>3,103</td>
</tr>
<tr>
<td>FLOPS count</td>
<td>184.7 PFLOP</td>
<td>33.2 PFLOP</td>
</tr>
</tbody>
</table>
Performance of AI-enhanced solver on K computer

- FLOP count decreased by 5.56-times from PCGE (standard solver; Conjugate Gradient solver with block Jacobi preconditioning) and 1.32-times from SC14 Gordon Bell Prize finalist solver (with multi-grid & mixed-precision arithmetic)

### Weak scaling

<table>
<thead>
<tr>
<th># of MPI processes (# nodes)</th>
<th>Developed</th>
<th>SC14</th>
<th>PCGE (Standard)</th>
</tr>
</thead>
<tbody>
<tr>
<td>576</td>
<td>1,951.2</td>
<td>3,774.1</td>
<td>36,398.1</td>
</tr>
<tr>
<td>1,152</td>
<td>3,774.1</td>
<td>3,774.1</td>
<td>18,908.7</td>
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<tr>
<td>2,304</td>
<td>3,774.1</td>
<td>3,774.1</td>
<td>9,508.8</td>
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<tr>
<td>4,608</td>
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<td>3,774.1</td>
<td>4,773.3</td>
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<td>9,216</td>
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<td>3,774.1</td>
<td>2,387.2</td>
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<tr>
<td>12,288</td>
<td>3,774.1</td>
<td>3,774.1</td>
<td>1,065.7</td>
</tr>
<tr>
<td>24,576</td>
<td>3,774.1</td>
<td>3,774.1</td>
<td>531.4</td>
</tr>
<tr>
<td>49,152</td>
<td>3,774.1</td>
<td>3,774.1</td>
<td>271.7</td>
</tr>
</tbody>
</table>

(17.2% of FP64 peak)

### Strong scaling

![Strong scaling graph](image-url)

- Elapsed time (s)
- # of MPI processes (# of nodes)
- Developed
- SC14
- PCGE (Standard)
Porting Strategy

• Our algorithm exhibits good performance/scalability on CPU-based supercomputer

• Same algorithm can be effective on GPU-based systems…?
  • Already designed for good scalability
  • Arithmetic count is reduced by AI in the solver
Requirements for Summit

- Inter-node throughput of Summit is relatively lower than previous supercomputer

- To attain higher performance, we have to reduce point-to-point communication cost more carefully
  - We have been using FP32-FP64 variables
  - Transprecision computing is available due to adaptive preconditioning

<table>
<thead>
<tr>
<th></th>
<th>K computer</th>
<th>Piz Daint</th>
<th>Summit</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU/node</td>
<td>1 × SPARC64 VIIIfx</td>
<td>1 × Intel Xeon E5-2690 v3</td>
<td>2 × IBM POWER 9</td>
</tr>
<tr>
<td>GPU/node</td>
<td>-</td>
<td>1 × NVIDIA P100 GPU</td>
<td>6 × NVIDIA V100 GPU</td>
</tr>
<tr>
<td>Peak FP32 performance/node</td>
<td>0.128 TFLOPS</td>
<td>9.4 TFLOPS</td>
<td>93.6 TFLOPS</td>
</tr>
<tr>
<td>Memory bandwidth</td>
<td>512 GB/s</td>
<td>720 GB/s</td>
<td>5400 GB/s</td>
</tr>
<tr>
<td>Inter-node throughput</td>
<td>5 GB/s in each direction</td>
<td>10.2 GB/s</td>
<td>25 GB/s</td>
</tr>
</tbody>
</table>
Introduction of FP16 variables

• Half precision can be used for reduction of data transfer size (Later used again in computation part)

  Single precision (FP32, 32 bits)  
  1bit sign + 8bits exponent + 23bits fraction

  Half precision (FP16, 16 bits)  
  1bit sign + 5bits exponent + 10bits fraction

• Using FP16 for whole matrix or vector causes overflow/underflow or fails to converge
  • Smaller exponent bits → small dynamic range
  • Smaller fraction bits → no more than 4-digit accuracy
FP16 for point-to-point communication

- FP16 MPI buffer only for boundary part
  - To avoid overflow or underflow, Original vector $\mathbf{x}$ is divided into one localized scaling factor $\text{Const}$ and FP16 vector $\bar{\mathbf{x}}^{16}$
- Data transfer size can be reduced
- $\text{Const} \times \bar{\mathbf{x}}^{16}$ does not match $\mathbf{x}$ exactly, but convergence characteristic is not changed for most problems
Overlap of computation and communication

1: \( r = Au \)  
2: \( \text{synchronize } q \text{ by point-to-point comm.} \)  
3: \( r = b - r; \ z = M^{-1}r \)  
4: \( \rho_a = 1; \ \alpha = 1; \ \rho_b = z \cdot r; \ \gamma = z \cdot q \)  
5: \( \text{synchronize } \rho_b, \gamma \text{ by collective comm.} \)  
6: \( \text{while } (|r_i|/|b_i| > \text{tolerance} ) \text{ do } \)  
7: \( \beta = -\gamma \rho_a / \alpha \)  
8: \( u = u + \alpha p; \ p = z + \beta p \)  
9: \( q = Ap \)  
10: \( \text{synchronize } q \text{ by point-to-point comm.} \)  
11: \( \rho_a = p \cdot q \)  
12: \( \text{synchronize } \rho_a \text{ by collective comm.} \)  
13: \( \alpha = \rho_b / \rho_a; \ \rho_a = \rho_b \)  
14: \( r = r - \alpha q; \ z = M^{-1}r; \ \rho_b = z \cdot r; \ \gamma = z \cdot q \)  
15: \( \text{synchronize } \rho_b, \gamma \text{ by collective comm.} \)  
16: \( \text{enddo} \)

- Conjugate Gradient method
- Introduce time-parallel algorithm
  - Solve four time steps in the analysis in parallel
  - Compute 1 current time step and 3 future time steps
  - Reduce iterations in the solver
- Computation becomes dense and suitable for low B/F architectures
Overlap of computation and communication

1': while (error_i > tolerance) do
2': Vector operation 1
3': Matrix vector multiplication
4': Point-to-point comm.
5': Vector operation 2
6': Collective comm.
7': Vector operation 3
8': Collective comm.
9': enddo

- Simplified loop
  - Computation part
    - 3 groups of vector operations
    - 1 sparse matrix vector multiplication
  - Communication part
    - 1 point-to-point communication
    - 2 collective communication

- Point-to-point communication is overlapped with matrix vector multiplication

PE#0: boundary part: send/receive between other MPI processes

inner part:
1. boundary part computation
2. inner part computation & boundary part communication

- However, this communication is still bottleneck of the solver
Overlap of computation and communication

- 4 vectors are divided into 2 vectors × 2 sets
- Point-to-point communication is overlapped with other vector operations
- The number of collective communication is unchanged

\[ \text{i, i+1-th time step} \]

1' : **while** (error\(_i\) > tolerance) **do**
2' :
3' : Collective comm.
4' : Vector operation 1
5' : Matrix vector multiplication
6' : Point-to-point comm.
7' : Vector operation 2
8' : Collective comm.
9' :
10' :
11' : Vector operation 3
12' : **endo**

\[ \text{i+2, i+3-th time step} \]

1' : **while** (error\(_i\) > tolerance) **do**
2' :
3' : Collective comm.
4' :
5' :
6' : Vector operation 3
7' :
8' : Collective comm.
9' : Vector operation 1
10' : Matrix vector multiplication
11' : Point-to-point comm.
12' : **endo**
Low precision variables for computation part in the solver

• Manage to reduce communication cost in the solver
• Now, it’s worth reducing computation cost to improve time-to-solution by using transprecision computing
  • FP21 for memory bound vector operations
  • FP16 for Element-by-Element kernel
    • Process $2 \times \text{FP16}$ variables on 2-element vector simultaneously and expect double performance
FP16 computation in Element-by-Element method

- Matrix-free matrix-vector multiplication
  - Compute element-wise multiplication
  - Add into the global vector

- Normalization of variables per element can be performed
  - To avoid underflow/overflow, we use values close to 1 in multiplication

\[
f = \sum_e P_e A_e P_e^\top u
\]

[\(A_e\) is generated on-the-fly]
Implementation of FP16 computation

- Vectors $u_e$ are scaled to avoid overflow/underflow in using half precision
- Element matrix $A_e$ is generated on-the-fly and also scaled
  - reorder computation ordering so that values close to 1 are used
- Most costly multiplication can be computed in FP16
- Achieved 71.9% peak FP64 performance on V100 GPU
Introduction of custom data type: FP21

- Most computation in CG loop is memory bound computation
  - However, it’s impossible to use FP16 for whole vector
- Trying to use FP21 variables for other memory bound computation

- Single precision (FP32, 32 bits)
  - 1bit sign + 8bits exponent + 23bits fraction

- FP21, 21 bits
  - 1bit sign + 8bits exponent + 12bits fraction

- Half precision (FP16, 16 bits)
  - 1bit sign + 5bits exponent + 10bits fraction
Implementation of FP21 computation

• Not supported in hardware, used only for storing
  • FP21(stored)⊢bit operation⇒FP32(computed)
• FP21 × 3 are stored into 64bit array
  • We are solving 3D finite element solver, so x, y, and z components can be stored as one components of 64 bits array
• 1/3 of memory consumption compared to FP64 variables
Performance measurement

On GPU-based supercomputer, Piz Daint and Summit
Performance comparison

- We solve the same problem as K-computer using 288 GPUs on Piz Daint & Summit
  - PCGE (conventional solver)
  - GAMERA (SC14 Gordon Bell Finalist solver)
  - MOTHRA (our proposed solver)
- MOTHRA is sufficiently faster than other solvers on Summit
  - 25.3-fold speedup from PCGE
  - 3.99-fold speedup from GAMERA
- Convergence characteristic is not largely changed even when we use FP16 & FP21
Weak scaling on Piz Daint

- MOTHRA demonstrates high scalability (89.5% to the smallest case)
  - Leading to 19.8% peak FP64 performance on nearly full system

<table>
<thead>
<tr>
<th># of GPUs</th>
<th>288</th>
<th>576</th>
<th>1152</th>
<th>2304</th>
<th>4608</th>
</tr>
</thead>
<tbody>
<tr>
<td># of node</td>
<td>288</td>
<td>576</td>
<td>1152</td>
<td>2304</td>
<td>4608</td>
</tr>
<tr>
<td>DOF</td>
<td>$3.5 \times 10^9$</td>
<td>$7 \times 10^9$</td>
<td>$14 \times 10^9$</td>
<td>$28 \times 10^9$</td>
<td>$56 \times 10^9$</td>
</tr>
<tr>
<td>MOTHRA’s efficiency to FP64 peak</td>
<td>22.1%</td>
<td></td>
<td></td>
<td></td>
<td>19.8%</td>
</tr>
</tbody>
</table>
Weak scaling on Summit

- Scalability greatly improves compared to previous solver GAMERA
- MOTHRA demonstrates high scalability
  - Leading to 14.7% peak FP64 performance on nearly full system
Summary and future implications

• Combination with FP16-FP21-FP32-FP64 transprecision computation/communication techniques enabled high performance of
  • 25.3-fold speedup from standard solver
  • 3.99-fold speedup from state-of-the-art SC14 Gordon Bell Finalist solver
  • 14.7% peak FP64 performance on near full system of Summit (4096 nodes)

• Co-design with those who understand architectures is critical to exhibit higher performance
Summary and future implications

• Integration of data analytics and equation based modeling is one of the key questions in high performance computing
  • New class of algorithms is required for accelerating equation based simulation by data analytics
  • We accelerated earthquake simulation by designing a scalable solver algorithm that can robustly incorporate data analytics
• Idea of accelerating simulations with data analytics can be generalized for other types of equation based modeling
  • Future development of high-performance computer systems supporting both data analytics and equation based simulations is key tool for advance of science and engineering
Acknowledgments

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