Scaling Out Alternating Direction Isogeometric L2 Projections Solver

Grzegorz Gurgul (AGH)
Bartosz Baliś (AGH)
Marcin Łoś (AGH)
Danuta Szeliga (AGH)
Maciej Paszyński (AGH)

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Agenda

- Background
- Isogeometric L2 projections solver - theory
- Isogeometric L2 projections solver - algorithm
- Isogeometric L2 projections solver - implementation
- Conclusions

Background

- Isogeometric L2 projections algorithm

Proposed by prof. Victor Calo: L. Gao, V.M. Calo, *Fast Isogeometric Solvers for Explicit Dynamics*, **Computer Methods in Applied Mechanics and Engineering** *(2014).*

- *Applications to time-dependent problems*

Non-linear flow (Fortran+MPI, parallel): M. Woźniak, M. Łoś, M. Paszyński, L. Dalcin, V. Calo, Parallel fast isogeometric solvers for explicit dynamics, **Computing and Informatics** *(2015)*

Tumor growth simulations (C++ sequential): M. Łoś, M. Paszyński, A. Kłusek, W. Dzwinel, Application of fast isogeometric L2 projection solver for tumor simulations, **Computer Methods in Applied Mechanics and Engineering** *(2017)*

Background

- Improving performance of time-dependent applications of ADS

Step 1: CUDA implementation:
G. Gurgul, M. Paszyński, W. Dzwinel, Łoś, *GPGPU accelerations of tumor growth simulation using isogeometric L2 - projections solver,* **USACM Conference on Isogeometric Analysis and Meshfree Methods** *(2016)*

Step 2: Object-Oriented shared memory implementation:
G. Gurgul, M. Paszyński, D. Szeliga, Open source JAVA implementation of the parallel multi-thread alternating direction isogeometric L2 projections solver for material science simulations, **Computer Methods in Material Science** *(2017)*

Step 3: Cloud implementation:
G. Gurgul, Bartosz Baliś, Marcin Łoś, D. Szeliga, M. Paszyński, Scaling Out Alternating Direction Isogeometric L2 Projections Solver, **14th U.S. National Congress on Computational Mechanics**

Isogeometric L^2 projections

In general: non-stationary problem of the form

$$\partial_t u - \mathcal{L}(u) = f(x,t) \implies \sum_{ij} u_{ij}(B_{ij}, B_{kl})_{L^2} = RHS$$

with some initial state u_0 and boundary conditions

$\mathcal{L}$ – well-posed linear spatial partial differential operator

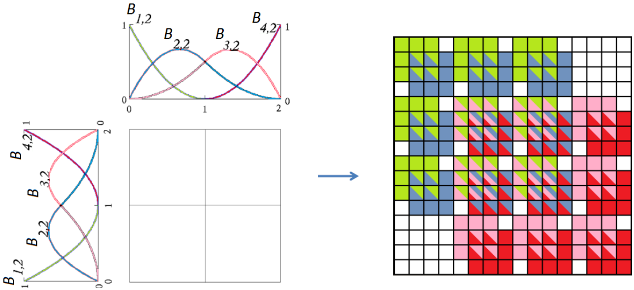
Discretization:

- spatial discretization: isogeometric FEM

  Basis functions: $\phi_1, \ldots, \phi_n$ (tensor product B-splines)

- time discretization with explicit method
- implies isogeometric L^2 projections in every time step

L^2 projections – tensor product basis



Isogeometric basis functions:

- 1D B-splines basis $B_1(x), \ldots, B_n(x)$
- higher dimensions: tensor product basis
  $B_{i_1 \cdots i_d}(x_1, \ldots, x_d) \equiv B_{i_1}^{x_1}(x_1) \cdots B_{i_d}^{x_d}(x_d)$

Gram matrix of B-spline basis on 2D domain $\Omega = \Omega_x \times \Omega_y$:

$$\mathcal{M}_{ijkl} = (B_{ij}, B_{kl})_{L^2} = \int_\Omega B_{ij} B_{kl} \, \mathrm{d}\Omega$$

L^2 projections – tensor product basis

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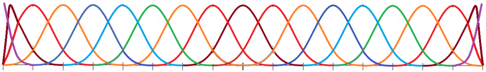
Gram matrix of B-spline basis on 2D domain $\Omega = \Omega_x \times \Omega_y$:

$$\begin{aligned}
\mathcal{M}_{ijkl} = (B_{ij}, B_{kl})_{L^2} &= \int_\Omega B_{ij} B_{kl} \, \mathrm{d}\Omega \\
&= \int_\Omega B_i^x(x) B_j^y(y) B_k^x(x) B_l^y(y) \, \mathrm{d}\Omega \\
&= \int_\Omega (B_i B_k)(x) \, (B_j B_l)(y) \, \mathrm{d}\Omega \\
&= \left(\int_{\Omega_x} B_i B_k \, \mathrm{d}x \right) \left(\int_{\Omega_y} B_j B_l \, \mathrm{d}y \right) \\
&= \mathcal{M}_{ik}^x \mathcal{M}_{jl}^y
\end{aligned}$$

$$\mathcal{M} = \mathcal{M}^x \otimes \mathcal{M}^y \quad \text{(Kronecker product)}$$



B-spline basis functions have **local support** (over $p+1$ elements)

$\mathcal{M}^x$, $\mathcal{M}^y$, ... – banded structure

$\mathcal{M}^x_{ij} = 0 \iff |i-j| > 2p+1$

Exemplary basis functions and matrix for cubics

$$\begin{bmatrix}
(B_1,B_1)_{L^2} & (B_1,B_2)_{L^2} & (B_1,B_3)_{L^2} & (B_1,B_4)_{L^2} & 0 & 0 & \cdots & 0 \\
(B_2,B_1)_{L^2} & (B_2,B_2)_{L^2} & (B_2,B_3)_{L^2} & (B_2,B_4)_{L^2} & (B_2,B_5)_{L^2} & 0 & \cdots & 0 \\
(B_3,B_1)_{L^2} & (B_3,B_2)_{L^2} & (B_3,B_3)_{L^2} & (B_3,B_4)_{L^2} & (B_3,B_5)_{L^2} & (B_3,B_6)_{L^2} & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots \\
0 & 0 & \cdots & (B_n,B_{n-3})_{L^2} & (B_n,B_{n-2})_{L^2} & (B_n,B_{n-1})_{L^2} & (B_n,B_n)_{L^2} &
\end{bmatrix}$$

Alternating Direction Solver – 2D

Two steps – solving systems with **A** and **B** in different *directions*

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & 0 \\ A_{21} & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{nn} \end{bmatrix} \begin{bmatrix} y_{11} & y_{21} & \cdots & y_{m1} \\ y_{12} & y_{22} & \cdots & y_{m1} \\ \vdots & \vdots & \ddots & \vdots \\ y_{1n} & y_{2n} & \cdots & y_{mn} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{21} & \cdots & b_{m1} \\ b_{12} & b_{22} & \cdots & b_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ b_{1n} & b_{2n} & \cdots & b_{mn} \end{bmatrix}$$

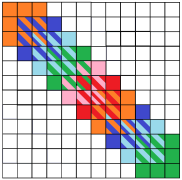
$$\begin{bmatrix} B_{11} & B_{12} & \cdots & 0 \\ B_{21} & B_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{mm} \end{bmatrix} \begin{bmatrix} x_{11} & \cdots & x_{1n} \\ x_{21} & \cdots & x_{2n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n} \\ y_{21} & y_{22} & \cdots & y_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m1} & y_{m2} & \cdots & y_{mn} \end{bmatrix}$$

Two one dimensional problems with multiple RHS:

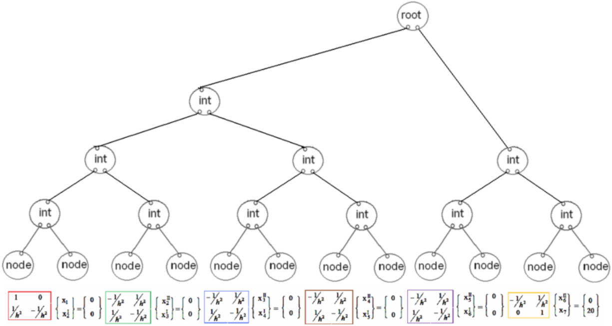
- $n \times n$ with m right hand sides $\rightarrow O(n * m) = O(N)$
- $m \times m$ with n right hand sides $\rightarrow O(m * n) = O(N)$

Linear computational cost $O(N)$ as opposed to $O(N^{1.5})$ or $O(N^2)$

The backing data structure is a tree. Each of its nodes holds coefficients of a simple linear equation being a portion of the original system.



Partition of the problem matrix into sub-matrices



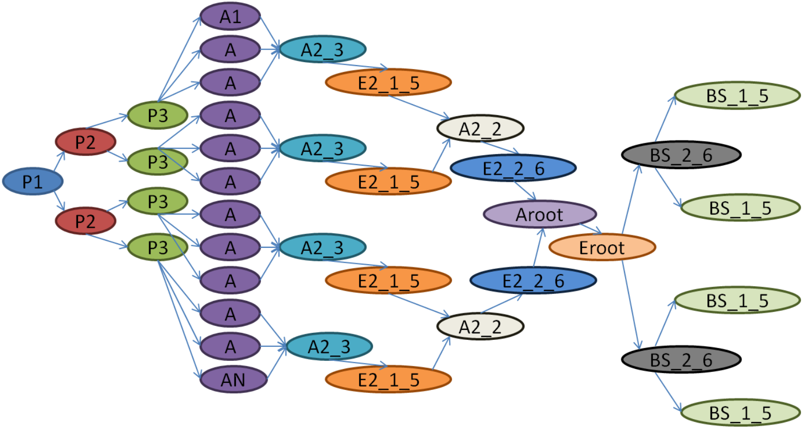
Graph of matrices the solver will operate on

Algorithm - set of operations

We can identify a set of basic tasks applicable on any vertex. We call them **productions**. They can:

- branch a vertex into two $\{P1, P2\}$ or three $\{P3\}$ child vertices
- initialize a vertex with particular coefficients $\{A1, A, AN\}$
- merge two vertices and eliminate unknowns - $\{A2\_3, E1\_2\_5, A2\_2, E2\_2\_6, Aroot, Eroot\}$
- backward substitute parts of solution - $\{BS\_2\_6, BS\_1\_5\}$

To obtain a solution for a 1-dimensional problem with 12 elements it is enough to execute the following productions, set by set, going from left to right, on respective vertices.



Implementation

CUDA (GPU):

- extremely fast for problems which *fit in on-board memory*
- verbose and fragile
- hardware dependent

Shared memory (Multicore CPU)

- fast for problems which fit in RAM (37 million elements require 16GB of RAM)
- portable, easy to understand and adapt
- scales up only

In memory grid (Cloud)

- can solve problems of any size
- slower for relatively small problems
- *scales out*

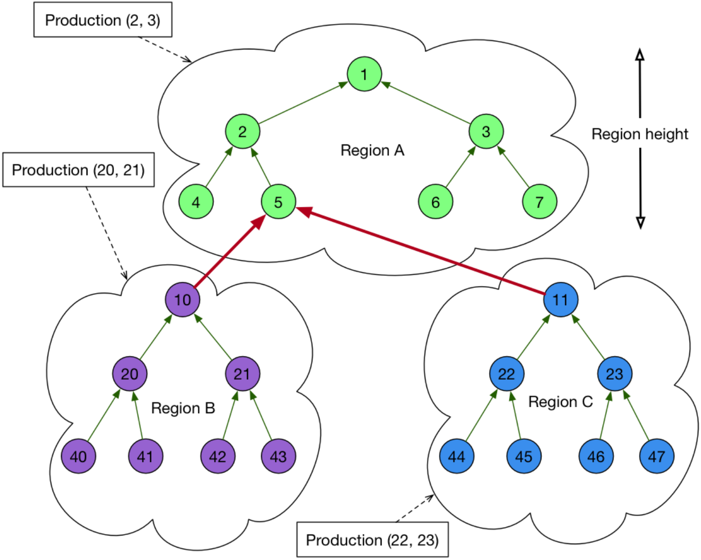
Implementation - performance considerations

Distributed environment implies *heavy network traffic* and increased memory consumption due to *extensive serialization*. This has to be reduced to the absolute minimum to let solver run bigger problems.

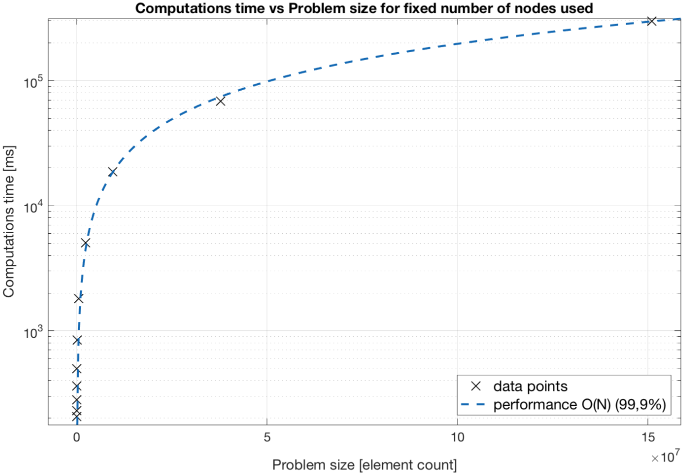
The following measures have been used:

- split tree into set of subtrees of a given height and store them on a single node
- use localized map-reduce to extract columns from the solution rows
- reuse same operation on multiple vertices
- run subsequent operations applied on same vertex in one invocation
- schedule tasks in batches
- use near-caches
- keep solution in deserialized form

Implementation - partition tree

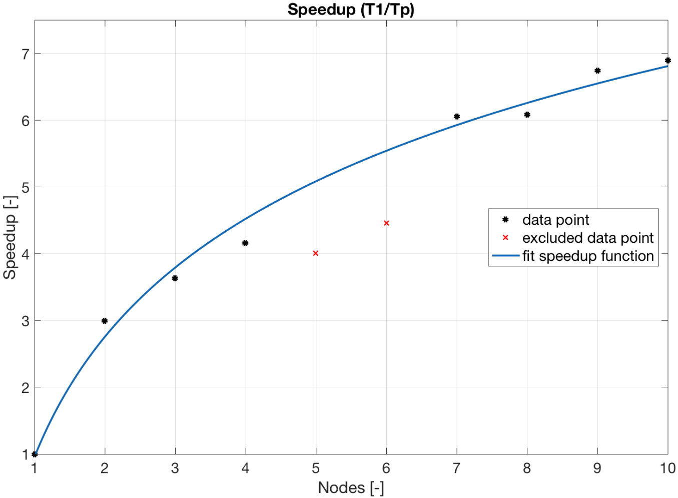


Implementation - time complexity - O(N)



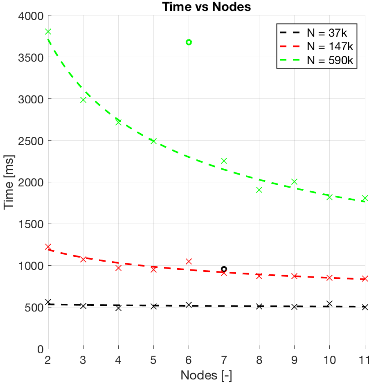
* Run on a cluster of 11 machines - Westmere (Nehalem-C 2.7GHz) CPU with 4 cores / 8GB RAM each

Implementation - speedup

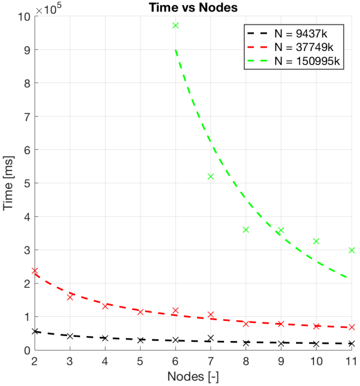


* Run for a fixed problem size. Each node has Westmere (Nehalem-C 2.7GHz) CPU with 4 cores / 8GB RAM each

Implementation - scaling out



Small problems (2m elem.)



Larger problems (2m to 150m elem.)

* Each node has Westmere (Nehalem-C 2.7GHz) CPU with 4 cores / 8GB RAM each

Conclusions

- Distributed memory implementation is slower than shared memory one for small problem sizes which fit into physical memory of a single machine
- It can solve any problem by adding additional nodes (4 - 6144, 6 - 12288, 12 - 24576)
- Given there is a shared memory machine with sufficient physical memory, IMDG implementation outperforms it starting from a certain problem size
- This implementation can be made significantly faster by pushing some logic into worker nodes

Thank you!

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