

Scaling Out Alternating Direction Isogeometric L2 Projections Solver

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**14th U.S. National Congress on Computational
Mechanics**

July 17-20, 2017, Montreal, Canada



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



- 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. Dzwiniel, *Application of fast isogeometric L2 projection solver for tumor simulations*, **Computer Methods in Applied Mechanics and Engineering** (2017)



- Improving performance of time-dependent applications of ADS

Step 1: CUDA 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*, **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**



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

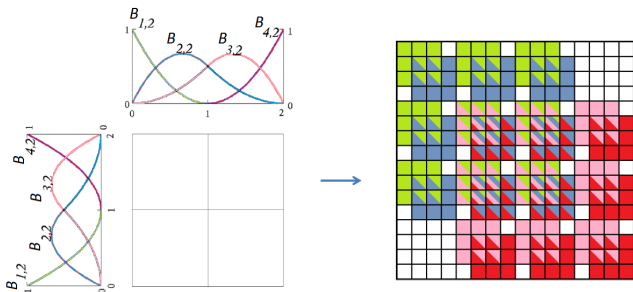
Discretization:

- spatial discretization: isogeometric FEM

Basis functions: ϕ_1, \dots, ϕ_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 $B_1(x), \dots, B_n(x)$
- higher dimensions: tensor product basis

$$B_{i_1 \dots i_d}(x_1, \dots, x_d) \equiv B_{i_1}^{x_1}(x_1) \cdots B_{i_d}^{x_d}(x_d)$$

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

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

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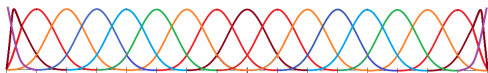
$$= \int_{\Omega} B_i^x(x) B_j^y(y) B_k^x(x) B_l^y(y) \, d\Omega$$

$$= \int_{\Omega} (B_i B_k)(x) (B_j B_l)(y) \, d\Omega$$

$$= \left(\int_{\Omega_x} B_i B_k \, dx \right) \left(\int_{\Omega_y} B_j B_l \, dy \right) \\ = \mathcal{M}_{ik}^x \mathcal{M}_{jl}^y$$

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

Gram matrix of tensor product basis



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

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

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

Exemplary basis functions and matrix for cubics

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

Alternating Direction Solver – 2D

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

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

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

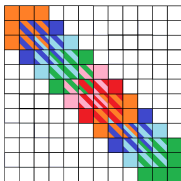
Two one dimensional problems with multiple RHS:

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

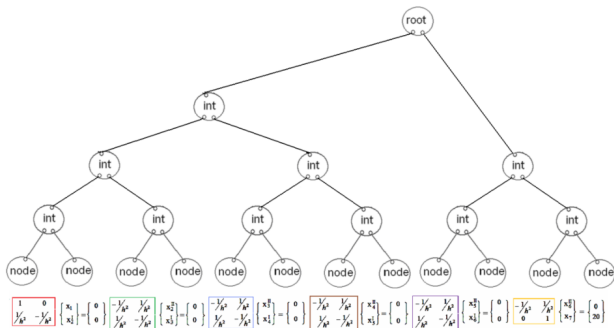
Linear computational cost $O(N)$ as opposed to $O(N^{1.5})$ or $O(N^2)$

Algorithm - data structure

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



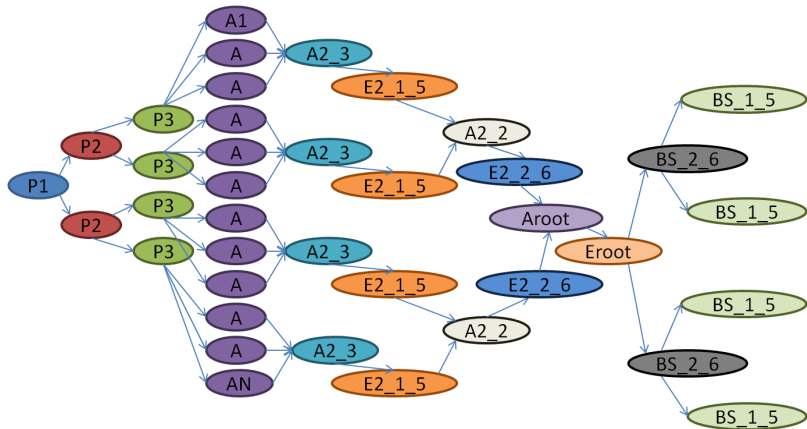
Graph of matrices the solver will operate on

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 - $\{BS_2_6, BS_1_5\}$

Algorithm - flow

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.



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*

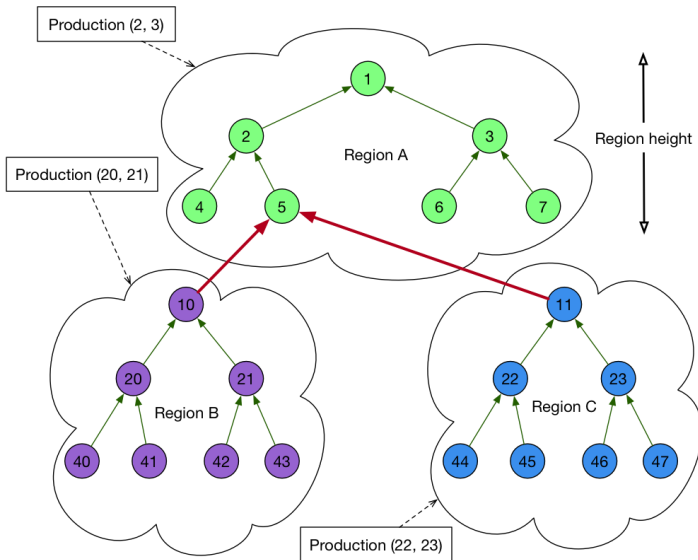
Implementation - performance considerations

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.

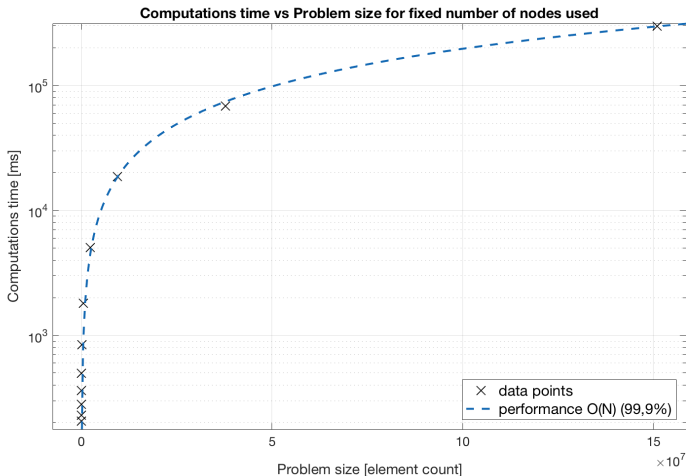
The following measures have been used:

- 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

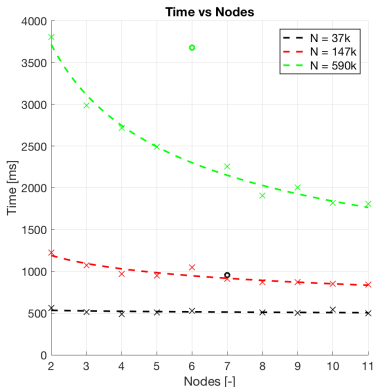


Implementation - time complexity - $O(N)$

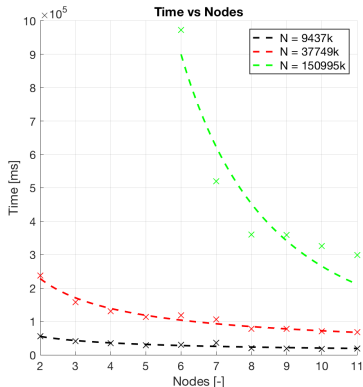


* Run on a cluster of 11 machines - Westmere (Nehalem-C 2.7GHz) CPU with 4 cores / 8GB RAM each

Implementation - 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

- 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!

Our research is supported from Dean's grant from Faculty of Computer Science, Electronics and Telecommunication, AGH University, Krakow, Poland