PARALLELIZATION OF A FINITE DIFFERENCE SCHEME FOR SOLVING SYSTEMS OF 2D SINE-GORDON EQUATIONS

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THE PROBLEM

A system of 2D perturbed Sine-Gordon equations is given:

$$S(\varphi_{tt} + \alpha\varphi_t + \sin\varphi - \gamma) = \Delta\varphi, \quad (x, y) \in \Omega \subset \mathbb{R}^2$$

Here S is the $N \times N$ cyclic tridiagonal matrix

$$S = \begin{pmatrix} 1 & s & 0 & . & 0 & s \\ s & 1 & s & 0 & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & 0 & s & 1 & s \\ s & . & 0 & 0 & s & 1 \end{pmatrix}$$

Neumann boundary conditions are considered:

$$\frac{\partial\varphi}{\partial\vec{n}}|\partial\Omega = 0$$

The unknown is the column vector $\varphi = (\varphi_1, ..., \varphi_N)^T$.
Parameters are $-0.5 < s \leq 0, \quad 0 < \alpha < 1, \quad \gamma > 0$.

COMPUTATIONAL CHALLENGES

We investigate a system of 2D differential equations.

In some cases the computational domain size may be very large
- $\mathbf{10^6 - 10^8}$ mesh points.

Also in some cases a very long time integration is needed
- $\mathbf{10^8 - 10^9}$ time steps.
Actually the number of time steps depend on parameters $\boldsymbol{s}$ and $\boldsymbol{\alpha}$.

$\Rightarrow$ Serious computational resources are needed!

THE GOALS OF THE WORK

The goals of the work are:

1.To make OpenMP realization of a difference scheme for solving systems of 2D perturbed Sine-Gordon equations.

2. To test the performance scalability of the OpenMP program on the CPU part of one computational node in the HybriLIT cluster and on one node of the CPU platform in the IICT-BAS cluster.

3. To multiply the parallelization effect by a domain decomposition and fully hybrid strategy: one MPI process per cluster node and OpenMP on the cores of the node.
(If good OpenMP performance scalability inside one node is achieved)

4. To test the performance scalability of the Hybrid MPI+OpenMP program on multiple nodes in the CPU platform in the IICT-BAS cluster.

THE FINITE DIFFERENCE SCHEME

We consider rectangular domains and introduce uniform rectangular mesh of size $\boldsymbol{h}$ and fixed time step of size $\boldsymbol{\tau}$.

Using second order centered finite differences for both time and space derivatives, we achieve our scheme.

As a result, at every interior mesh point we need to solve a system of one and the same cyclic tridiagonal matrix $\boldsymbol{S}$. We use Gaussian elimination. The cost is only $\boldsymbol{9N-12}$ floating point operations. The diagonally dominance of the matrix ($\boldsymbol{-0.5 < s \leq 0}$) ensures the stability of the Gaussian elimination.

THE STABILITY CONDITION

The von Neumann (linear) stability condition is:

$$\tau < \frac{\sqrt{1+2s} \quad h}{\sqrt{2}}$$

τ - the step in time

h - the mesh size of the uniform rectangular mesh

$\sqrt{1+2s} = \sqrt{\lambda_{min}}$ where λ_{min} is the minimal eigenvalue of S

$\sqrt{2}$ in the denominator corresponds to dimension = 2

THE ENERGY EQUALITY

We need to check the following energy equality:

$$\frac{d}{dt}E(t) + \alpha \iint_{\Omega} (\sum_{i=1}^{N} \varphi_{i,t}^2)\, dx\, dy = 0$$

where

$$E(t) = \iint_{\Omega} \frac{1}{2}(\varphi_x^T S^{-1} \varphi_x + \varphi_y^T S^{-1} \varphi_y) +$$

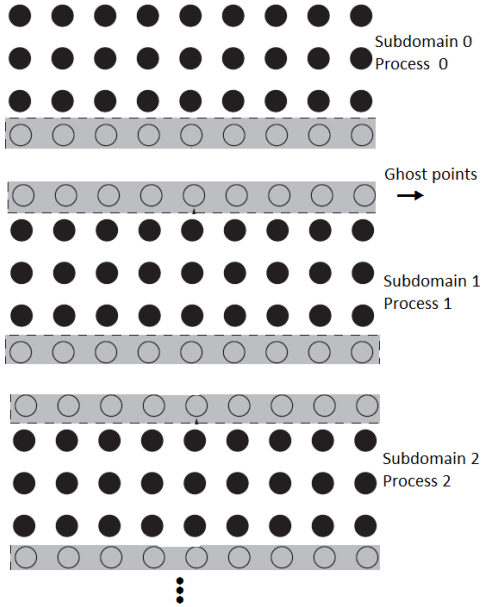
$$+ \sum_{i=1}^{N} (\frac{1}{2}\varphi_{i,t}^2 + 1 - cos\varphi_i - \gamma\varphi_i)\, dx\, dy$$

Parallelization strategy: Fully hybrid MPI+OpenMP

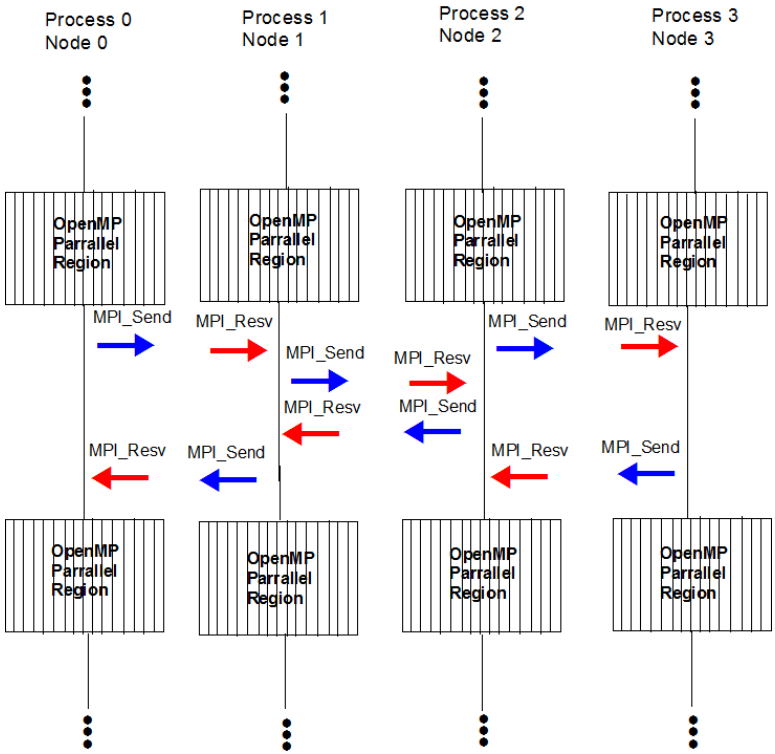
We make domain decomposition with one MPI process working on one cluster node. Ghost points are introduced to support the receives between MPI processes.

Inside a subdomain the work is shared between OpenMP threads. At every mesh point a system with the matrix $\boldsymbol{S}$ is solved.

Only master threads communicate (outside the parallel OpenMP region).



Parallelization strategy: Fully hybrid MPI+OpenMP
Fork-Join model + Ordered Sends and Receives in paires

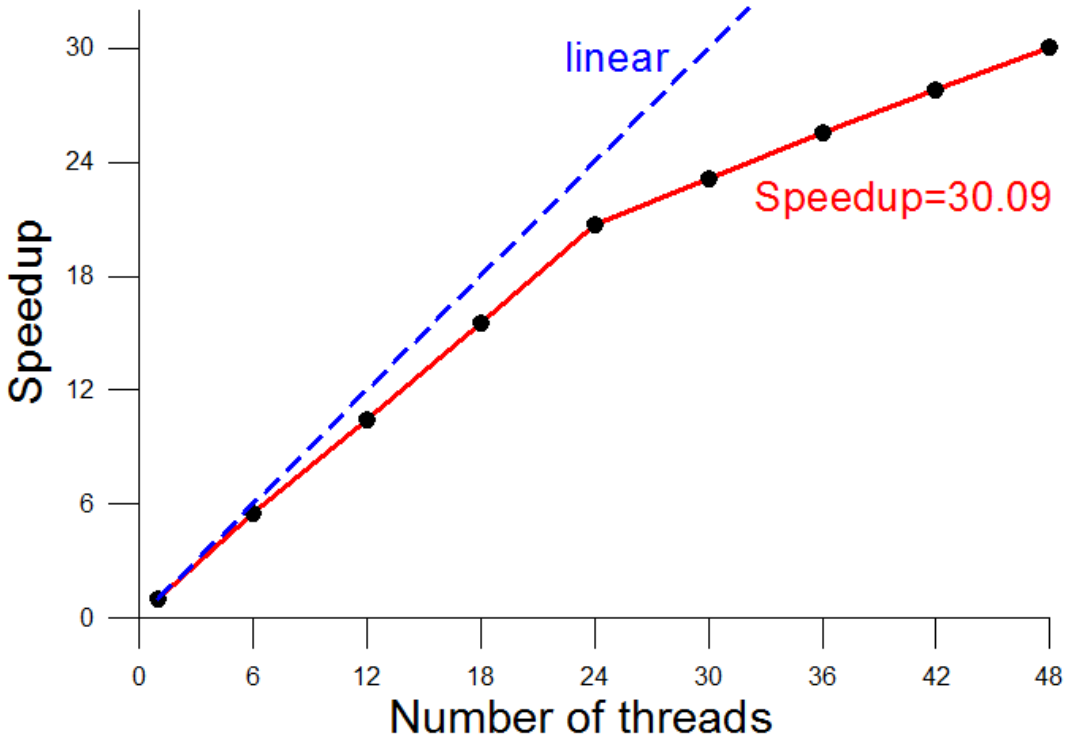


OpenMP performance in HybriLIT

Scatter thread affinity is used. The threads are distributed as evenly as possible across the entire system.
For most OpenMP codes, scatter should provide the best performance, as it minimizes cache and memory bandwidth contention.
In the following table computational domain size is:
$\boldsymbol{N_{eq}} \times \boldsymbol{N_x} \times \boldsymbol{N_y} = \mathbf{10} \times \mathbf{3000} \times \mathbf{3000} = \mathbf{9.10^7}$, $\boldsymbol{N_{time}} = \mathbf{300}$.
The test in double precision arithmetic is done on the CPU part of one node in the HybriLIT cluster, i.e. on
2 x ***Intel*®** ***Xeon*®** Processors E5-2695 v2 (24 cores, 48 threads).

Number of threads	Time (seconds)	Speedup	Parallel efficiency (%)
1	549.97	1.00	100.
6	99.87	5.51	91.8
12	52.79	10.42	86.8
18	35.33	15.57	86.5
24	26.54	20.72	86.3
30	23.75	23.16	77.2
36	21.51	25.57	71.0
42	19.75	27.85	66.3
48	18.28	**30.09**	62.7

OpenMP performance scalability inside one node

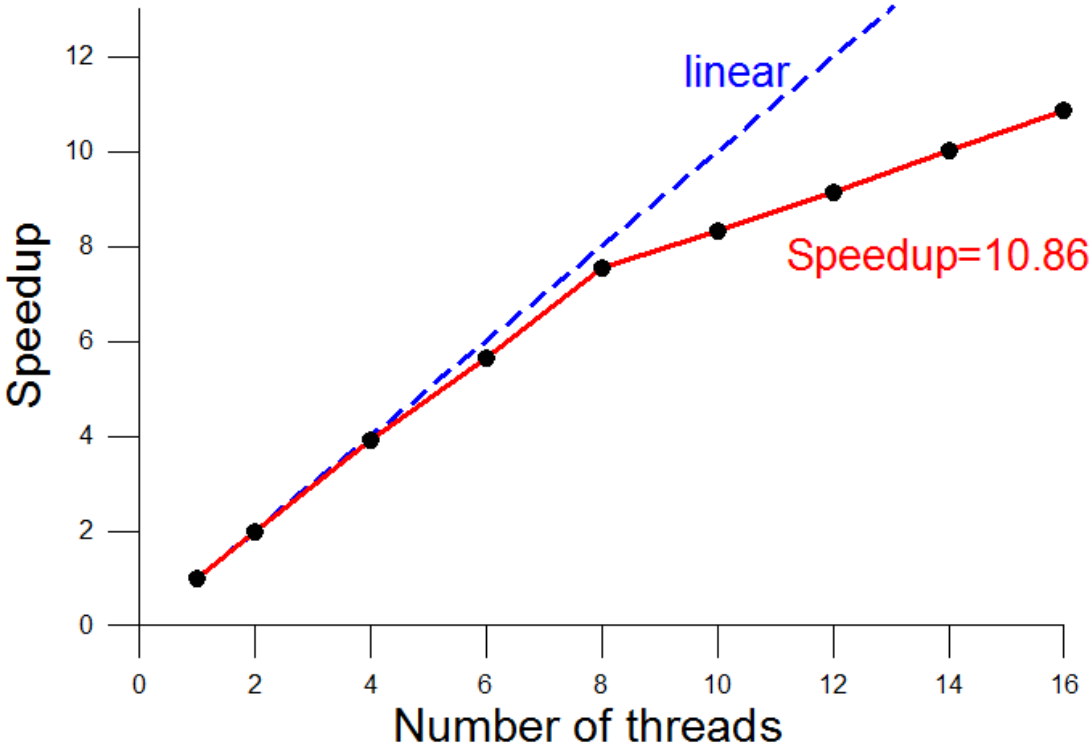


OpenMP performance on the CPU platform of IICT-BAS cluster

In the following table computational domain size is:
$\boldsymbol{N_{eq}} \times \boldsymbol{N_x} \times \boldsymbol{N_y} = \mathbf{10} \times \mathbf{3600} \times \mathbf{3600} \sim \mathbf{13.10^7}$,
$\boldsymbol{N_{time\_steps}} = \mathbf{150}$.
The test in double precision arithmetic is done on one node of the CPU platform of the IICT-BAS cluster :
2 x ***Intel*®** ***Xeon*®** Processors X5560 (8 cores, 16 threads).

Number of threads	Time (seconds)	Speedup	Parallel efficiency (%)
1	411.49	1.00	100.
2	208.92	1.97	98.4
4	105.08	3.92	97.9
6	72.76	5.66	94.3
8	54.58	7.54	94.2
10	49.31	8.34	83.4
12	44.91	9.16	76.3
14	41.07	10.02	71.6
16	37.88	**10.86**	67.9

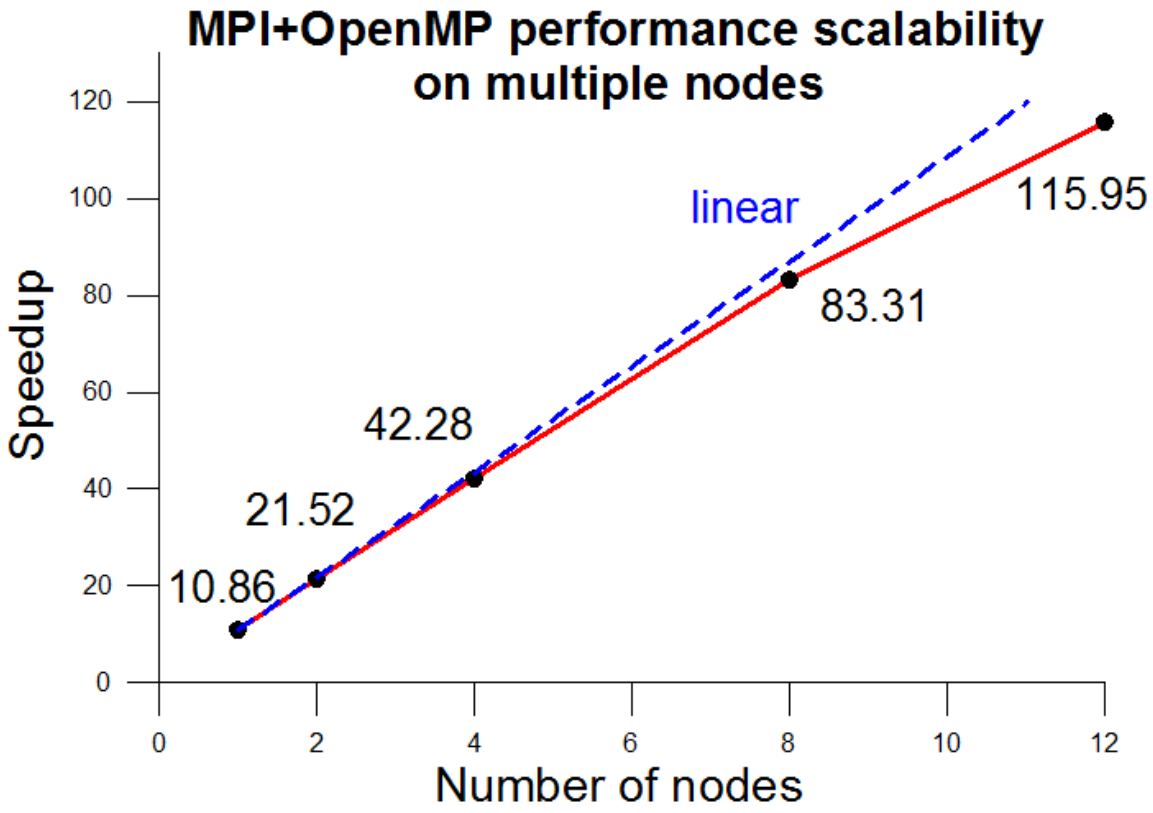
OpenMP performance scalability inside one node



MPI+OpenMP performance on multiple nodes in the CPU platform of the IICT-BAS cluster

In the following table only N_{time_steps} is changed: $N_{time\_steps} = 1800$.

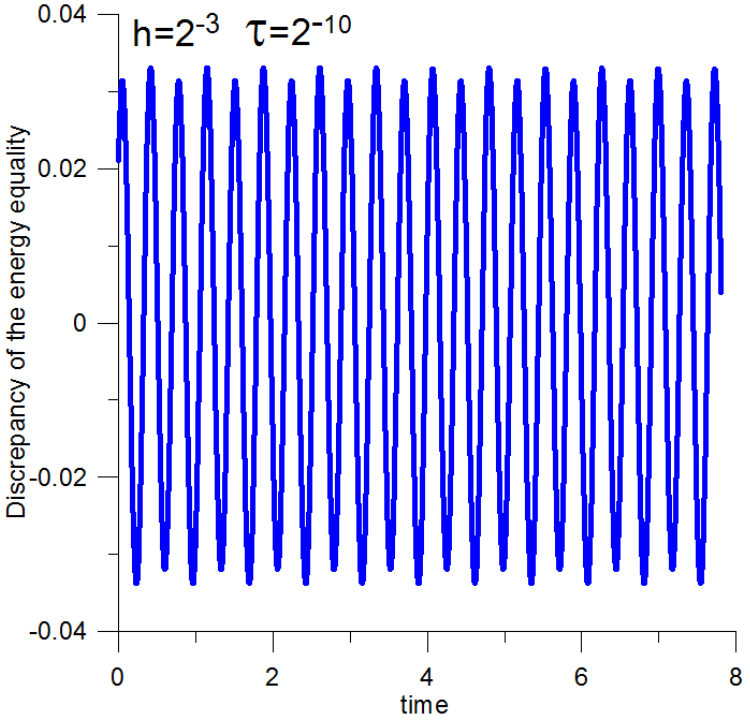
Number of nodes	Time (seconds)	Speedup	Relative to one node efficiency (%)
1	454.50	10.86	100.
2	229.34	21.52	99.1
4	116.72	42.28	97.3
8	59.25	83.31	95.9
12	42.57	**115.95**	89.0


MPI+OpenMP performance scalability
on multiple nodes
Speedup
Number of nodes
linear
10.86
21.52
42.28
83.31
115.95
0
20
40
60
80
100
120
0
2
4
6
8
10
12

SIMULATION EXAMPLE –

Nonlinear standing wave solution in 30x30 square,
4 equations, $\alpha = 0.13$, $\gamma = 1.14$, $s = -0.49993$.

Discrepancy of the energy equality



THANK YOU FOR YOUR ATTENTION!