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Periodic Orbits with “4D”

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Space-Time "4D" Approach

Transient Simulation of: $\mathbf{B}\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \lambda)$

First solve: $\mathbf{B}\frac{\mathbf{x}_1 - \mathbf{x}_0}{\Delta t} - \mathbf{f}(\mathbf{x}_1, \lambda) = 0$

Then solve: $\mathbf{B}\frac{\mathbf{x}_2 - \mathbf{x}_1}{\Delta t} - \mathbf{f}(\mathbf{x}_2, \lambda) = 0$

Then solve: $\mathbf{B}\frac{\mathbf{x}_3 - \mathbf{x}_2}{\Delta t} - \mathbf{f}(\mathbf{x}_3, \lambda) = 0$

Instead, solve for all solutions at once:

$$\mathbf{g}(\mathbf{y}, \lambda) = 0$$

where

$$\mathbf{y} = \begin{vmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \\ \mathbf{x}_5 \end{vmatrix}$$

$$\mathbf{g}_i = \mathbf{B}\mathbf{x}_i - \mathbf{B}\mathbf{x}_{i-1} - \Delta t \mathbf{f}(\mathbf{x}_i, \lambda)$$

… and with Newton solve:

$$\begin{vmatrix} (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 & 0 & 0 \\ -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 & 0 \\ 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 \\ 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 \\ 0 & 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) \end{vmatrix} \begin{vmatrix} \Delta\mathbf{x}_1 \\ \Delta\mathbf{x}_2 \\ \Delta\mathbf{x}_3 \\ \Delta\mathbf{x}_4 \\ \Delta\mathbf{x}_5 \end{vmatrix} = \begin{vmatrix} -\mathbf{g}_1 \\ -\mathbf{g}_2 \\ -\mathbf{g}_3 \\ -\mathbf{g}_4 \\ -\mathbf{g}_5 \end{vmatrix}$$

$$"\mathbf{K}\Delta\mathbf{y} = -\mathbf{g}"$$

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Why do a Space-Time "4D" Approach?

1. Design: Formulating transient problems as "steady" problems in space-time allows for use:
   - Continuation
   - Adding Design Constraints
   - Optimization (Optimal control)
2. Scalability: Can implement parallelism over time domain
3. Periodic Orbits: Only way with analytic Jacobian
4. Verification: Can do mesh refinement in 1D time axis

- There are many potential hurdles and liabilities with this approach (high memory usage, poor scalability, incompatibility with mesh adaptivity, time step control,...)

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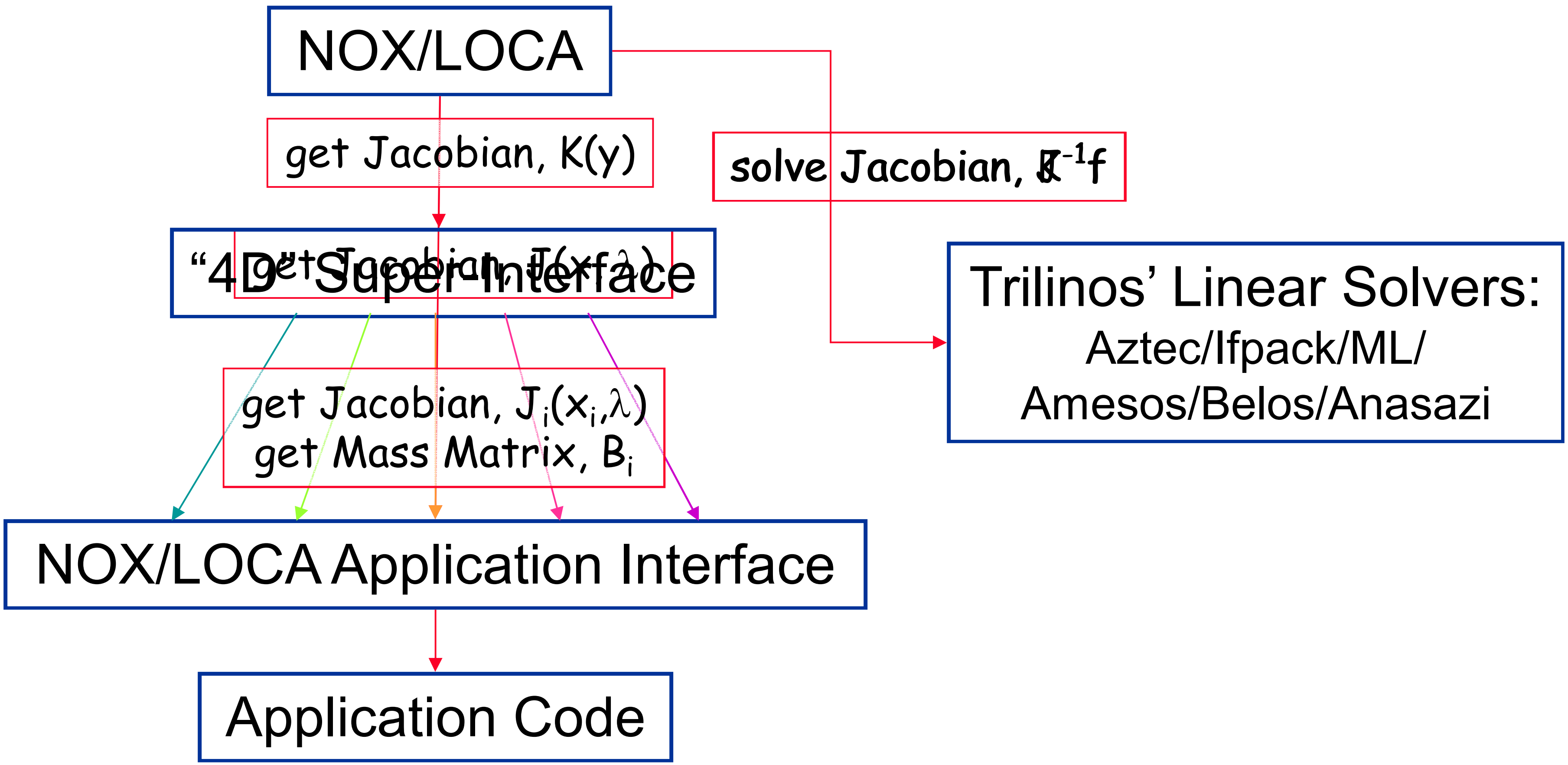
Trilinos Implementation of Space-Time Capability: create a "Super" NOX/LOCA interface



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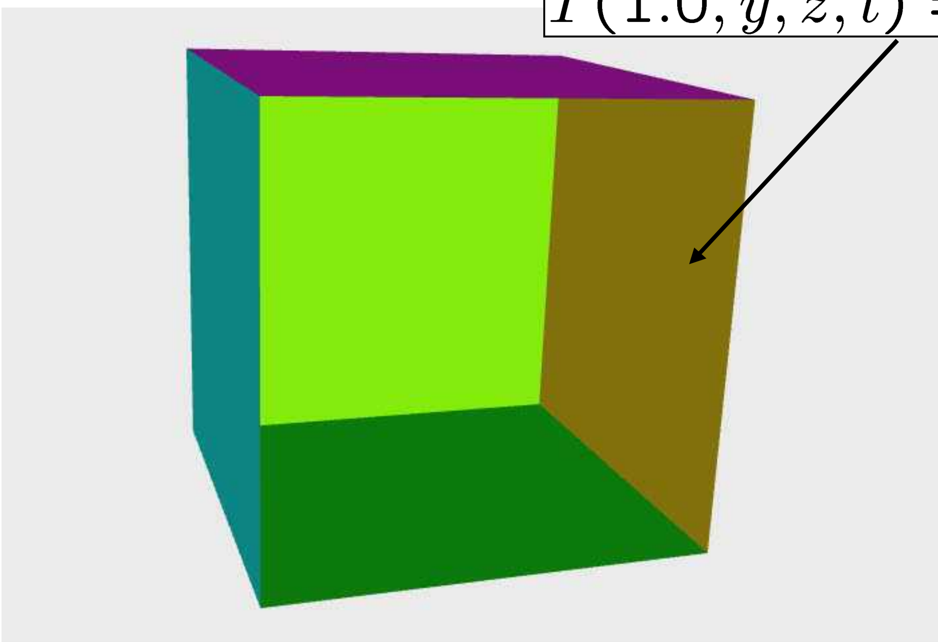
Periodic Solutions of Large Problems

$$\begin{vmatrix} (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 & 0 & -\mathbf{B} \\ -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 & 0 \\ 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 \\ 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 \\ 0 & 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) \end{vmatrix} \begin{vmatrix} \Delta\mathbf{x}_1 \\ \Delta\mathbf{x}_2 \\ \Delta\mathbf{x}_3 \\ \Delta\mathbf{x}_4 \\ \Delta\mathbf{x}_5 \end{vmatrix} = \begin{vmatrix} -\mathbf{g}_1 \\ -\mathbf{g}_2 \\ -\mathbf{g}_3 \\ -\mathbf{g}_4 \\ -\mathbf{g}_5 \end{vmatrix}$$

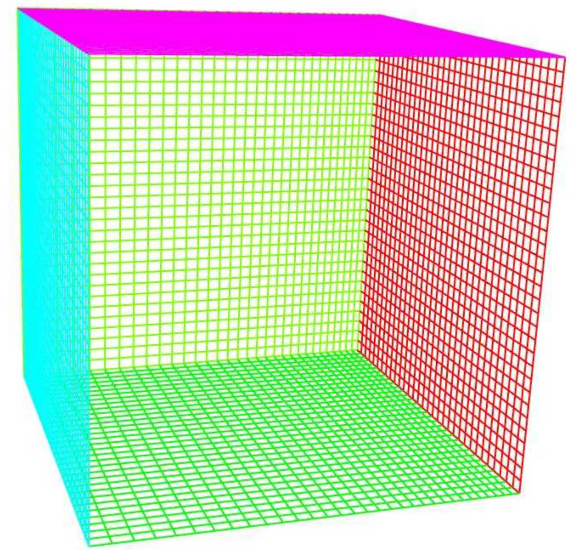
Demonstration Problem

3D Buoyancy-driven flow in a box with periodic thermal forcing

$$T(1.0, y, z, t) = sin(2\pi t)$$



MPSalsa



32 x 32 x 32 x 32 grid, with 5 PDEs

(32 x 32 x 32: F.E.; x 32: F.D.)

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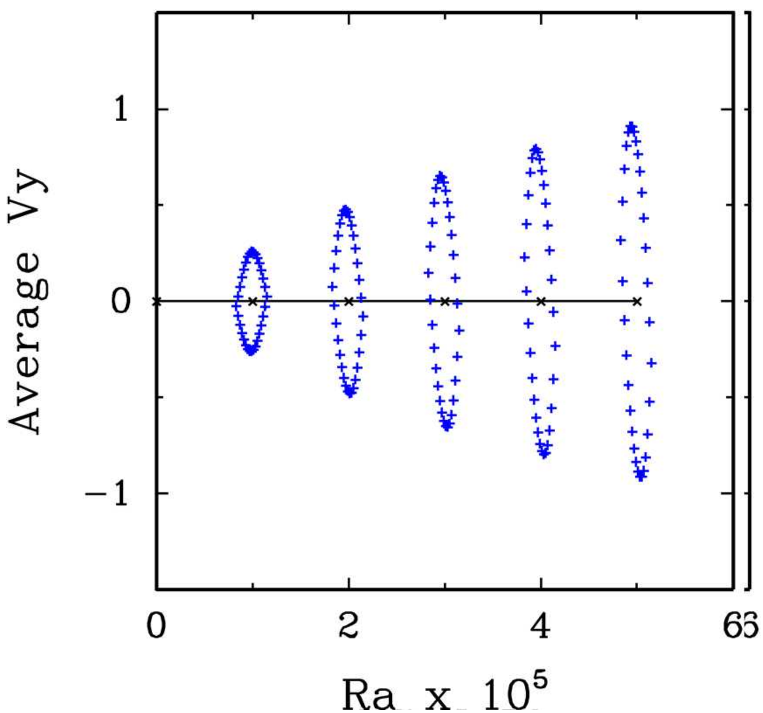
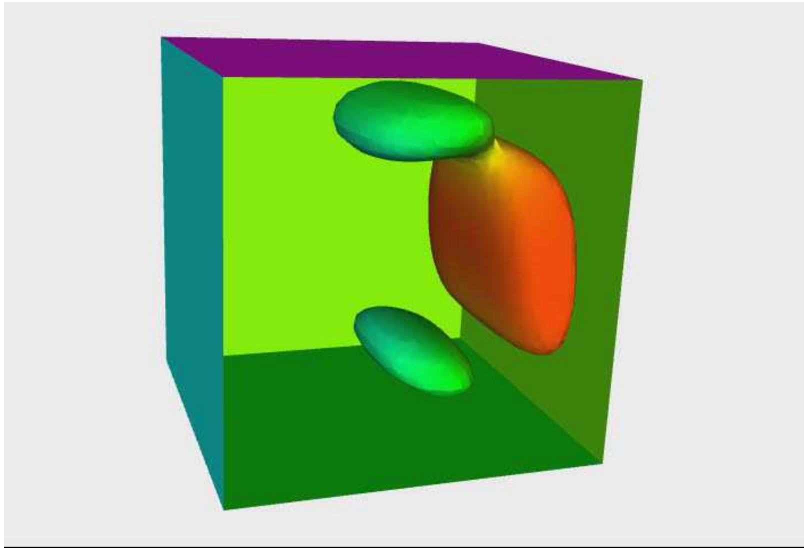
Demonstration Problem: Continuation Run

Ra (Rayleigh Number) = Buoyancy force compared to dissipation





Demonstration Problem: Timings

32 x 32 x 32 x 32 grid, with 5 PDEs = 5.75M unknowns,
(with 270 nonzeroes/row)

```
--------------XYZT Partition Info----------------
        NumProcs                   = 64
        Spatial Decomposition      = 2
        Number of Time Domains     = 32
        Time Steps on Domain 0     = 1
        Number of Time Steps       = 32
        -->Solving for a Periodic Orbit!
-----------------------------------------------
```

Preconditioner calc (ifpack): 31 sec
GMRES: 23 – 130 iters, 9 – 75 secs
Newton iters: 3-5
Continuation steps: 4
Total time: 30 min

Floquet Analysis of Periodic Orbit

Floquet Multipliers:

- Given a periodic solution
- Integrate perturbations through 1 period
- Eigenvalues of this operator are called Floquet Multipliers σ_i
- Orbits are stable if all $\|\sigma_i\| < 1$

- Arnoldi iteration of eigensolver:

$$\begin{vmatrix} (\mathbf{B}-\Delta t\mathbf{J}) & 0 & 0 & 0 & 0 \\ -\mathbf{B} & (\mathbf{B}-\Delta t\mathbf{J}) & 0 & 0 & 0 \\ 0 & -\mathbf{B} & (\mathbf{B}-\Delta t\mathbf{J}) & 0 & 0 \\ 0 & 0 & -\mathbf{B} & (\mathbf{B}-\Delta t\mathbf{J}) & 0 \\ 0 & 0 & 0 & -\mathbf{B} & (\mathbf{B}-\Delta t\mathbf{J}) \end{vmatrix} \begin{vmatrix} \ldots \\ \ldots \\ \ldots \\ \ldots \\ \mathbf{v}_{i+1} \end{vmatrix} = \begin{vmatrix} \mathbf{Bv}_i \\ 0 \\ 0 \\ 0 \\ 0 \end{vmatrix}$$

Where does the code currently reside?

packages/epetraext/src/block:
- EpetraExt::BlockVector
- EpetraExt::BlockCrsMatrix
- EpetraExt::MultiMpiComm

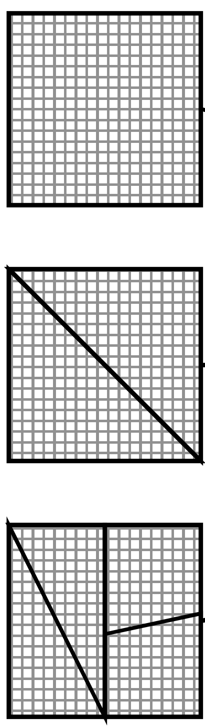
packages/nox/src-loca/src-epetra:
- LOCA::Epetra::Interface::xyzt
- LOCA::Epetra::xyztPrec
- LOCA::Epetra::AnasaziOperator::Floquet*

packages/nox/examples/epetra/LOCA_Brusselator_xyzt:
- Example.C

*Floquet capability only in development branch

Space and Time can be partitioned independently, Ex: 4 Time Steps on 4 Procs

Spatial Partition

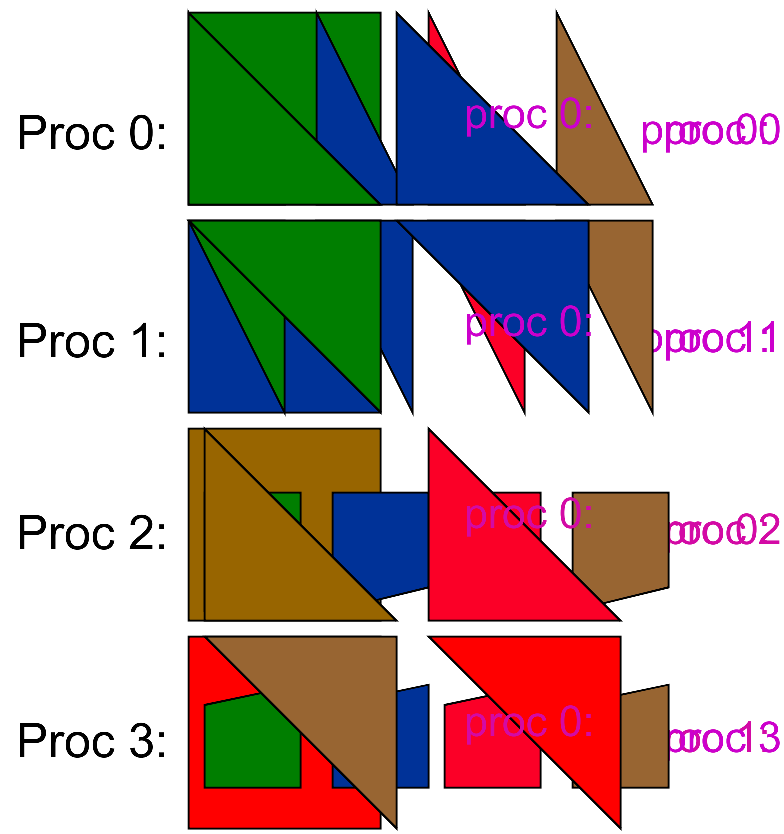


Each processor owns 1 time step for the entire spatial domain

Each processor owns 2 time steps for $\frac{1}{2}$ of the spatial domain

Each processor owns 4 time steps for $\frac{1}{4}$ of the spatial domain

Space-Time Partition



mpirun -np 4 salsa infile 4 4

Numerical Experiment #1

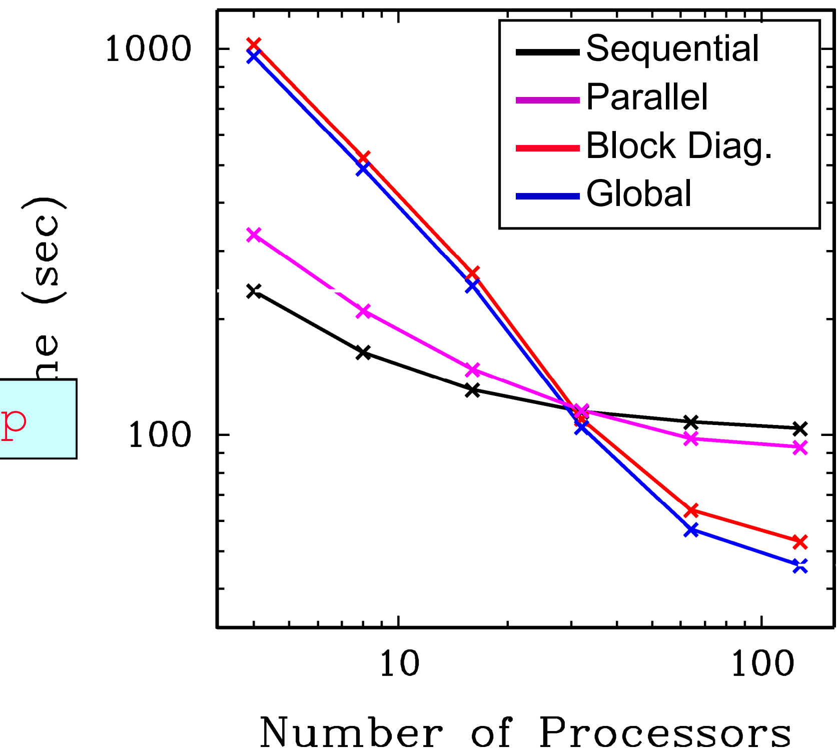
How much can parallelism in time speed up the solve?

- **Fixed Number of Spatial Domains (4)**
  - **Processors: 4 8 16 32 64 128**
  - **Time Domains: 1 2 4 8 16 32**

MPSalsa:
PDEs: 5
FEM: 2D, 64 x 48 elements
Time steps: 32
Unknowns: 509,600

Trilinos:
Newton (NOX) : 3-6 iterations
GMRES (Aztec) : <200 iters
ILUk (Ifpack) : overlap=0, fill=1
Continuation steps (LOCA): 1

5x Speedup



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Numerical Experiment #2

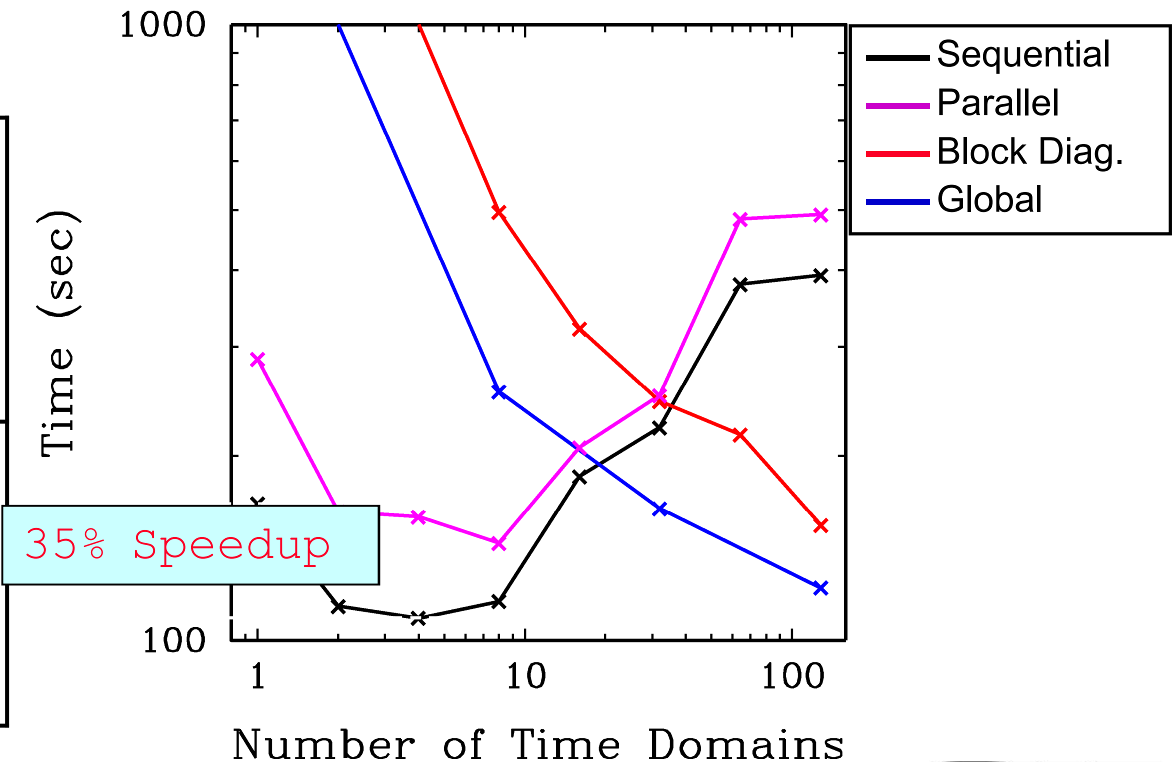
Can space-time parallelism be more effective than just spatial parallelism?

- **Fixed Number of Processors (128)**

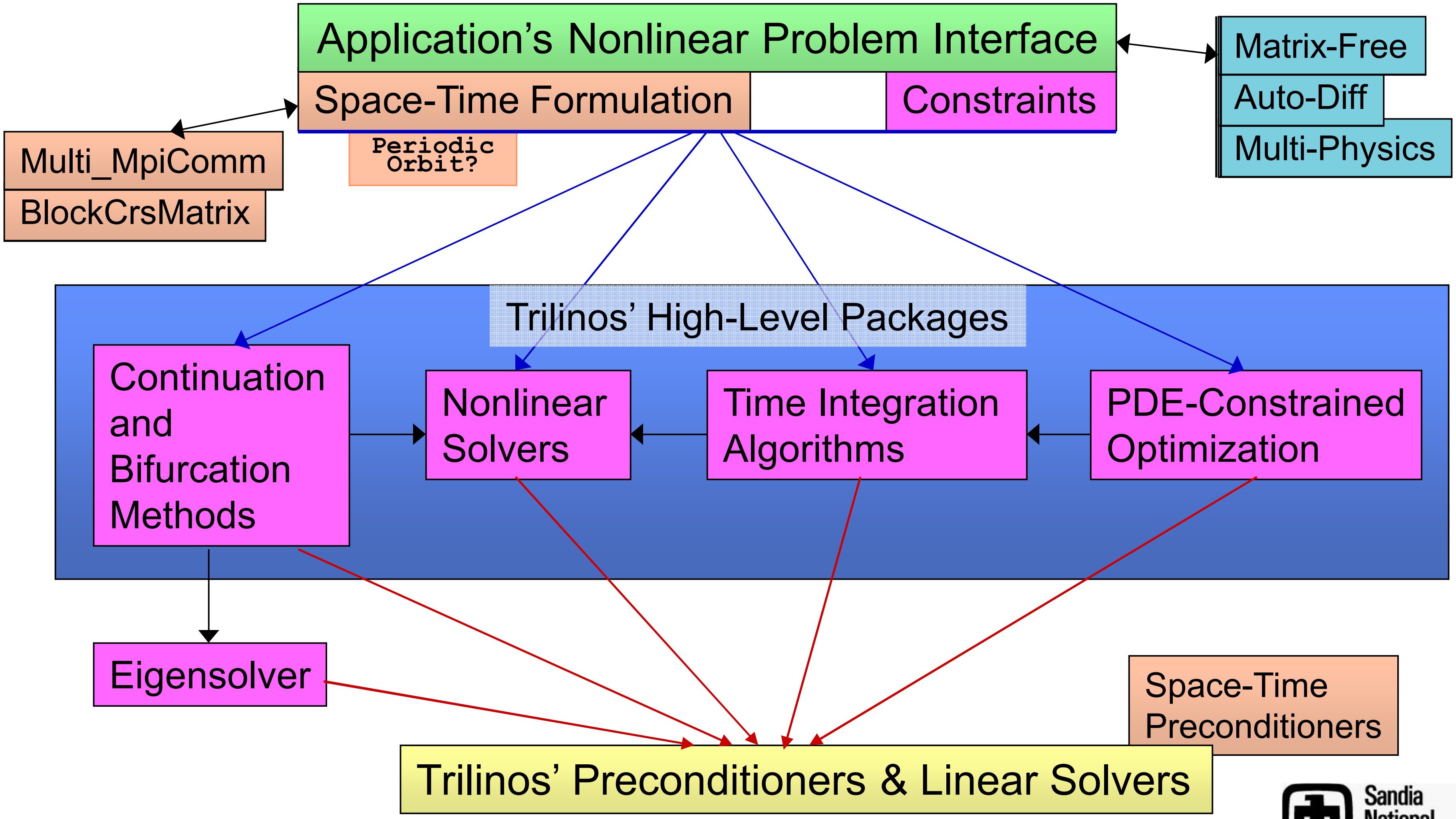
– Spatial domains:	1	2	4	8	16	32	64	128
– Time domains:	128	64	32	16	8	4	2	1

MPSalsa:
PDEs: 5
FEM: 2D, 64 x 48 elements
Time steps: 128
Unknowns: 2,038,400

Trilinos:
Newton (NOX) : 4–6 iterations
GMRES (Aztec) : <200 iters
ILUk (Ifpack) : overlap=0, fill=1
Continuation steps (LOCA): 1



Space-Time capability is integrated with Trilinos’ design and analysis tools



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