Non-linear Systems and Parallelization

Gundolf Haase

Karl-Franzens University Graz

Graz, Dec 2024

Bidomain equations with elasticity coupling

The coupling of mechanics with the bidomain is done via additional parameters **a** and **C** which lead to the modified bidomain equations

$$\begin{aligned}
-\nabla\cdot\boldsymbol{\sigma}_e\mathbf{C}^{-1}\nabla\phi_e &= \nabla\cdot\boldsymbol{\sigma}_i\mathbf{C}^{-1}\nabla\phi_i + I_e \\
\beta I_m &= \nabla\cdot\boldsymbol{\sigma}_i\mathbf{C}^{-1}\nabla\phi_i
\end{aligned}$$

$$\begin{aligned}
I_m &= C_m\frac{\partial V_m}{\partial t} + I_{ion}(V_m,\boldsymbol{\eta},\mathbf{a}) - I_i \\
\frac{d\boldsymbol{\eta}}{dt} &= f(t,\boldsymbol{\eta},\mathbf{a}) \\
V_m &= \phi_i - \phi_e
\end{aligned}$$

The coupling parameter **a** contains quantities calculated from the deformation model [Pathmanathan/Whiteley 2009], with the equilibrium equations of large elastic deformations describing the mechanic behavior,

Large elastic deformations

$$\begin{aligned}
-\mathrm{div}\ \sigma(u) &= f \quad , \\
\text{with:} \qquad \text{stress tensor} \quad \sigma &= 2J^{-1}F\frac{\partial\Psi(C)}{\partial C}F^\top \\
\text{deformation gradient tensor} \quad F_{ij} &= \frac{\partial x_i}{\partial X_j} \\
\text{compressible} \quad J &= \det F \quad \neq 1 \\
\text{Cauchy-Green deformation tensor} \quad C &= F^\top F,
\end{aligned}$$

where

$$\Psi = U(J) + \overline{\Psi}_{\text{iso}} + \overline{\Psi}_{\text{aniso}} + \overline{\Psi}_{\text{act}}(\boldsymbol{a}, \eta(V_m)), \quad U(J) = \frac{\kappa}{2}(J-1)^2 \ .$$

is the Helmholtz free energy both the isotropic and anisotropic response, an active part due to the excitation–induced contraction during the course of depolarization.

[Kroon/Holzapfel 2009; Pathmanathan/Whiteley 2009]

Non-linear elasticity: a sketch

We have to solve the non-linear (quasi-linear) system of equations

$$K(u) \cdot u = f$$

with deformation u via Newton iteration.
Per Newton step we have to solve

$$A'(u) \cdot \partial u = g(u) \tag{1}$$

with a priori accumulation of

$$\begin{aligned} A'(u) &:= \frac{\partial K(u)}{\partial u} \cdot u + K(u) \\ g(u) &:= f - K(u) \cdot u \end{aligned} \tag{2}$$

Non-linear elasticity: algorithmic view I

In each Newton iteration step we have to perform:

1. Generate $A'(u)$, $g(u)$
2. Solve (1) with PCG
    1. Setup of AMG-preconditioner
        1. Find coarse/fine nodes
        2. Calculate interpolation
        3. Calculate coarse grid operators
    2. Apply AMG-PCG
3. Update $\widehat{u} = u + \partial u$
4. Goto 1

Non-linear elasticity: algorithmic view I

In each Newton iteration step we have to perform:

1. Generate $A'(u)$, $g(u)$
2. Solve (1) with PCG
    1. Setup of AMG-preconditioner
        1. Find coarse/fine nodes
        2. Calculate interpolation
        3. Calculate coarse grid operators
    2. Apply AMG-PCG
3. Update $\widehat{u} = u + \partial u$
4. Goto 1

Take into account:

- matrix computation/accumulation might consume 50% of overall time (expensive operations to determine occupancy pattern of sparse matrices)
- memory transfer CPU $\leftrightarrow$ GPU is expensive

Non-linear elasticity: algorithmic view I

In each Newton iteration step we have to perform:

1. Generate $A'(u)$, $g(u)$
2. Solve (1) with PCG
    1. Setup of AMG-preconditioner
        1. Find coarse/fine nodes
        2. Calculate interpolation
        3. Calculate coarse grid operators
    2. Apply AMG-PCG
3. Update $\widehat{u} = u + \partial u$
4. Goto 1

Take into account:

- matrix computation/accumulation might consume 50% of overall time (expensive operations to determine occupancy pattern of sparse matrices)
- memory transfer CPU $\leftrightarrow$ GPU is expensive

$\Longrightarrow$ Move more computations and data onto the GPU.

Non-linear elasticity: algorithmic view II

1. Setup of operators (once)
    1. Calculate sparse pattern of $K(u)$, $A'(u)$ ($\longrightarrow$ patterns)
    2. Calculate $K(u)$, $A'(u)$, $g(u)$
    3. Setup of AMG-preconditioner wrt. $A'(u)$ ($\longrightarrow$ patterns)
2. Solve (1) with PCG (each iteration)
    1. Setup of AMG-preconditioner wrt. $A'(u)$ fixed sparsity pattern of operators
        1. Update interpolation
        2. Update coarse grid operators
        3. no setup
    2. Apply AMG-PCG
3. Update $\widehat{u} = u + \partial u$
4. Update $K(\widehat{u})$, $A'(\widehat{u})$, $g(\widehat{u})$ (fixed sparsity pattern)
5. Goto 2

Non-linear elasticity: algorithmic view III

1. Setup of operators
    1. Calculate sparse pattern of $K(u)$, $A'(u)$
    2. Calculate $K(u)$, $A'(u)$, $g(u)$ GPU: Costa (✓)
    3. Setup of AMG-preconditioner wrt. $A'(u)$ ($\longrightarrow$ patterns)
2. Solve (1) with PCG
    1. Setup of AMG-preconditioner wrt. $A'(u)$
       fixed sparsity pattern of operators
        1. Update interpolation GPU: Neic ✓
        2. Update coarse grid operators GPU: Neic ✓
        3. no setup
    2. Apply AMG-PCG GPU: done ✓
3. Update $\widehat{u} = u + \partial u$ GPU: Costa
4. Update $K(\widehat{u})$, $A'(\widehat{u})$, $g(\widehat{u})$ (fixed sparsity pattern) GPU: Costa (✓)
5. Goto 2

Local calculation of stiffness matrix (potential)

- Xeon E5645 with 6 cores; 2.4 GHz, 12MB of cache; 32 GB/sec bandwidth
- GTX 680 with 1536 CUDA cores, 1006 MHz Base Clock; 192.2 GB/sec memory bandwidth.
- `nvcc -O3` ; `gcc -O3`
- tetrahedrons with linear test functions

n elements	Std. vs. Vectorized	Vectorized vs. CUDA	Std. vs.CUDA
12.500	6.3	34	214
50.000	5.3	67	353
112.500	5.4	76	410
450.000	4.9	**84**	**416**
1.250.000	5.5	74	408

Table: Speedup (wrt. one CPU-core) of calculating the local stiffness matrices.

Global assembling of stiffness matrix on CPU/GPU

Assume: known pattern of global stiffnes matrix (CSR; done in setup once)
Two approaches:

1. store all element matrix entries globally into one large array (coord);
   - perfect parallel computation (vectorized)
   - precomputed accumululation pattern (from setup)
   - global accumulation is perfectly parallel
   - ? memory transfer — Liebmann/Neic [LN]
2. store local matrices only temporarily (or not at all); accumulate directly into global matrix
   $\longrightarrow$ offset information per element needed [DUNE also]
   - saves memory accesses
   - !! ressource conflicts when global matrix entries are updated
     $\Longrightarrow$ coloring of elements — Haase/Hraßnigg [HH]

Matrix assembling - OpenMP: May 9, 2014

Timing in sec.; 2 Mill. tetrahedra, linear test functions, potential problem
Workstation with Xeon E5-2600 v2, 10 cores

cores	LN	HH coloring	HH reord.	HH atomic $+=$	HH LN-array
1	0.88+0.51	1.80	1.06	**1.04**	0.82+0.51
2	0.80+0.26	1.08	**1.01**	1.04	0.75+0.26
4	0.70+0.22	0.67	0.41	**0.41**	0.36+0.22
10	0.68+0.10	0.53	**0.34**	0.39	0.28+0.10
20	0.54+0.05	0.36	0.33	**0.27**	0.23+0.05

Conclusion: **Atomic** operations are so **fast**, and potental conflicts so less, that **coloring doesn't pay off**
— at least for the test environment.

Matrix assembling - OpenMP: July 7, 2014

Timing in sec.; 15 Mill. tetrahedra, linear test functions, potential problem
Workstation with Xeon E5-2600 v2, 10 cores

	LN	HH	HH
cores		coloring	atomic $_{+=}$
1	7.3	**3.9**	5.5
2	4.6	**2.9**	3.4
4	3.6	2.4	**2.4**
8	2.8	2.4	**2.2**
10	3.3	2.3	**2.2**
20	4.9	1.8	**1.7**

Conclusion: **Atomic** operations are so **fast**, and potental conflicts so less, that **coloring doesn't pay off**

Implementation LN suffers much more from bandwidth saturation.
HH (atomic) is still an older code version.

Matrix assembling - OpenACC [since PGI 15.10]

```
#pragma acc kernels pcopyout(sk[0:nnz],f[0:nnode]),
                    pcopyin(ia[0:ndof_e*nelem],xc[0:2*nnode],id[0:nnode+1],ik[0:nnz])
   {
      const int idn = id[nnode];
#pragma acc loop
      //for (int k = 0; k < id[nnode]; ++k)  {   // will not be parallelized
      for (int k = 0; k < idn; ++k)  {           //      but this will parallelize
            sk[k] = 0.0; }
#pragma acc loop
      for (int k = 0; k < nnode; ++k)  {
            f[k] = 0.0; }

      float ske[3][3], fe[3];
#pragma acc loop private(ske,fe) vector(32)
      for (int i = 0; i < nelem; ++i) {
            CalcElem(ia + 3 * i, xc, ske, fe);
            AddElem(ia+3*i, ske, fe, id, ik, sk, f);
    }
    return;
}
```

Matrix assembling - OpenACC cnt.

```
#pragma acc routine seq
void CalcElem(const int ial[3], const float xc[], float ske[3][3], float fe[3])
{
   // sequ. code for one element
}


#pragma acc routine seq
void AddElem(const int ial[3], const float ske[3][3], const float fe[3],
             const int id[], const int ik[], float sk[], float f[])
{
#pragma acc loop                                 // needed [PGI 15.10]
    for (int i = 0; i < 3; ++i) {
        const int ii  = ial[i];
#pragma acc loop                                 // needed [PGI 15.10]
        for (int j = 0; j < 3; ++j) {            // no symmetry
            const int jj = ial[j];
            const int ip = fetch(ii, jj, id, ik);
#pragma acc atomic update                 // no atomic possible in seq—routine before PGI 15.5
            sk[ip] += ske[i][j];
        }
#pragma acc atomic update                 // no atomic possible in seq—routine before PGI 15.5
        f[ii] += fe[i];
    }
}
```

What about Xeon Phi?

Xeon Phi 60 cores (1GHz), 8 GB vs.2×Xeon E5-26508 (2GHz), 2×8 Cores

No MIC pragmas needed: OpenMP 4.0 fully in Intel compiler included

- Quantum mechanics, 1024 × 1024 points, 6 dimensions
- OpenMP on Host as well as on MIC (**native** mode)
- AVX and AVX2 vectorization in work for QR factorization.
- code by M. Liebmann / D. Sattlegger / M. Alinejadmofrad [May 9, 2014]

	Host		MIC			
cores	1	16	60	120	180	240
time(sec.)	41.4	**2.66**	6.6	3.8	2.9	**2.4**
efficiency	1.00	0.97	1.00	0.87	0.76	0.70

In progress

- **native** mode: all code and all data on MIC
- **offload** mode: explicit data transfer to/from MIC

Linear elasticity

Lamé equations: linear elasticity for small deformations $\left|\frac{\partial u_l}{\partial x_k}\right| << 1$

$$\begin{array}{rrll} & -\text{div}\ \sigma(u) & = f & , \\ \text{with:} & \text{stress tensor} & \sigma = & D\varepsilon := 2\delta_{i,j}\varepsilon_{i,i} + 2\mu\varepsilon_{i,j} \\ & \text{Cauchy deformation tensor:} & \varepsilon_{k,l} = & \frac{1}{2}\left(\frac{\partial u_l}{\partial x_k} + \frac{\partial u_k}{\partial x_l}\right) \end{array}$$

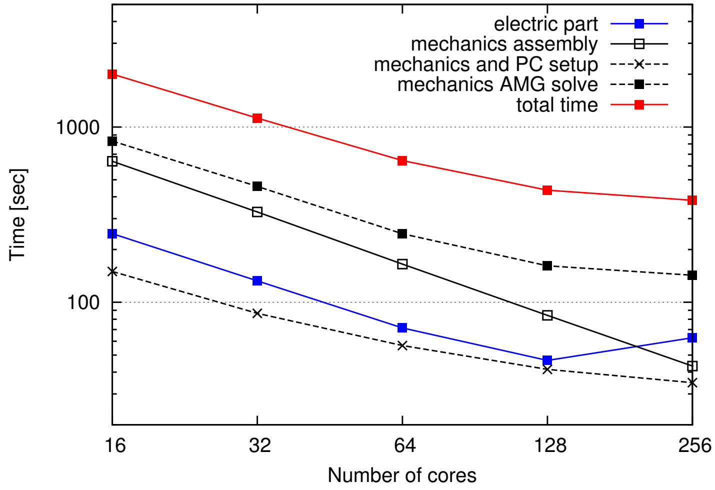
Tetrahedra with linear f.e. functions.

AMG components

- Coarsening by agglomeration regarding strong connections.
- Intergrid transfer by constant interpolation/averaging
  - matrix dependent intergrid transfer: less iterations but slower in sum
- Block (3×3) Jacobi-smoother
- still the older communicator
- still the old coarse grid parallelization

Example: elasticity + potential problem

TBunnyC: 862,515 vertices ($n + 3 \times n$ dofs) on CPU [GPU: $10\times$]



©C.Augustin