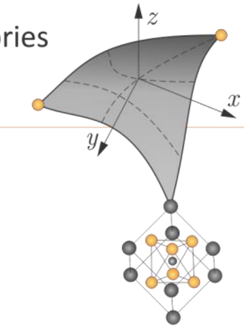

A Case Study on Design and Performance of a Generic Finite Element Library

Yingrui (Ray) Chang

Graduate Aerospace Laboratories
California Institute of Technology

Congress on Strange Mechanics
Weird Place, CA
February 31, 2013

Education & Experience

Yingrui (Ray) Chang
California Institute of Technology

Education:

- **Doctor of Philosophy (Ph.D.)** in Mechanical Engineering, 2010 - present
  Minor in CSE (Computational Science and Engineering)
  California Institute of Technology, CA.
- **Master of Science (M.S.)** in Computational Mechanics, 2009 - 2010
  Carnegie Mellon University, PA .
- **Bachelor of Engineering (B.E.)** in Civil Engineering, 2005 - 2009
  Tongji University, Shanghai, China.

Experience:

- **model building and solving:**
  - building and solving partial differential equations (**PDEs**) arising in mechanics and material science;
  - numerical PDEs, linear algebra, optimization, etc.
- **programming skills:**
  - building C++ numerical finite element (FEM) libraries for solving PDEs;
  - high-performance computing (MPI, openmp);
  - other languages: python, Java, C.

Magnesium and Magnesium Alloys

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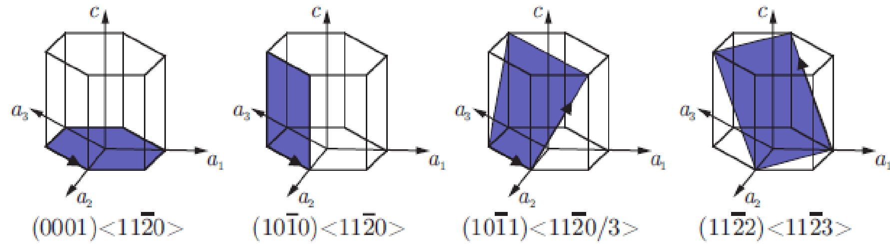
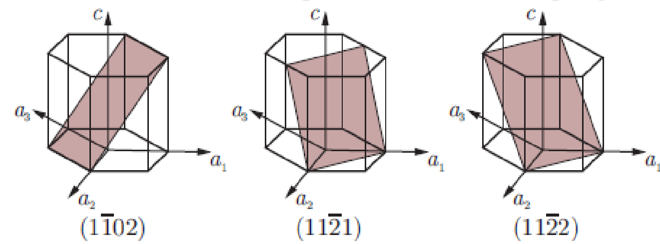
general properties:

atomic number: 12
melting point: 923 K (650 ˚C)
density: 1.738 g/cm^3
(Fe: $7.8 g/cm^3$; Al: 2.7 g/cm^3)
Young's modulus: 45 GPa
shear modulus: 17 GPa
crystal structure: hcp

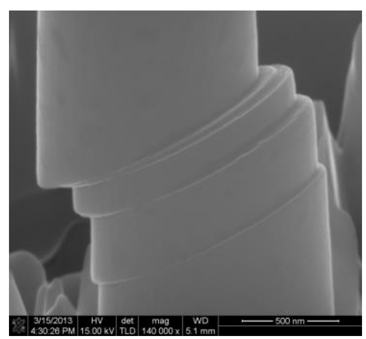
crystal plasticity: hcp slip systems



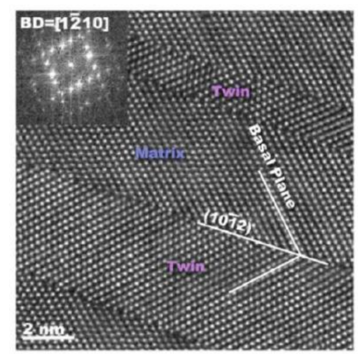
deformation twinning: hcp twinning systems



experimental evidence of twinning and slip in magnesium:



(Z. Aitken, J. Greer, 2014)



(Yu, Qi, Chen, Mishra, Li &Minor. 2011)

Building Models for Magnesium and Mg Alloys

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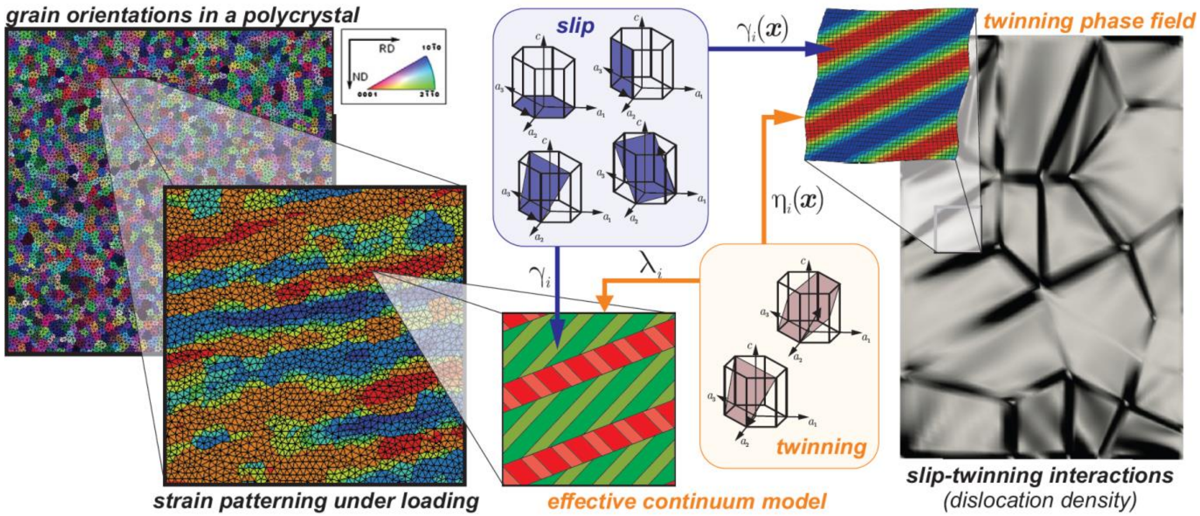
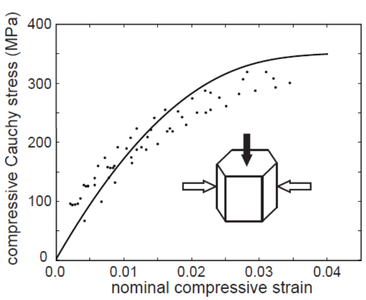
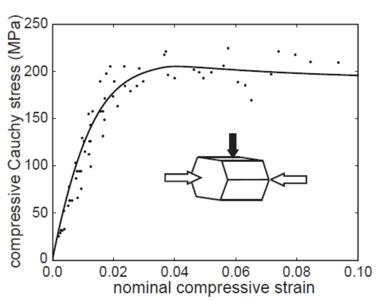
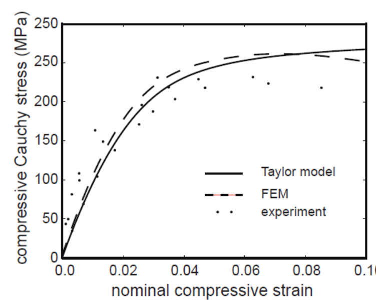
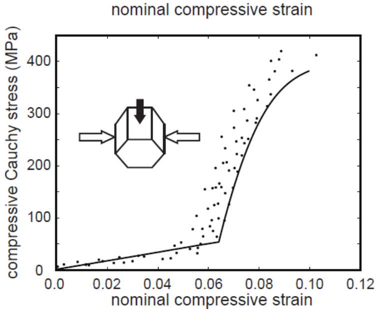


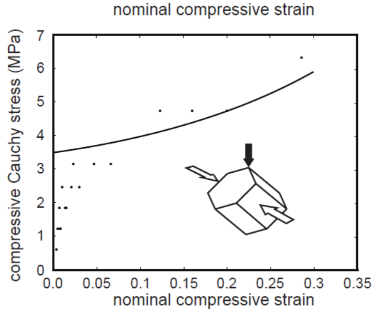
grain structure and FE mesh representation:



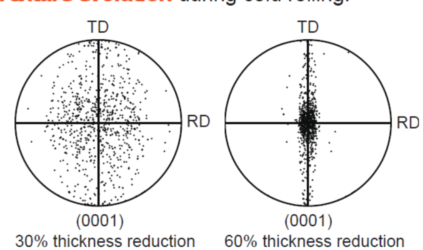








Texture evolution during cold rolling:



microstructure formation:

unpublished result here.

Presentation Outline

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California Institute of Technology

- **Brief introduction to finite element method (FEM):**
  - what problem we are solving;
  - FEM domain discretization;
  - role of **assembler class**;
- **Design study for building generic FEM code:**
  - inheritance (virtual function) approach;
  - template approach;
- **Performance study on threading FEM assembler class:**
  - assemble energy;
  - assemble force vector;
  - assemble tangent matrix.

Typical Model Building Flow Chart

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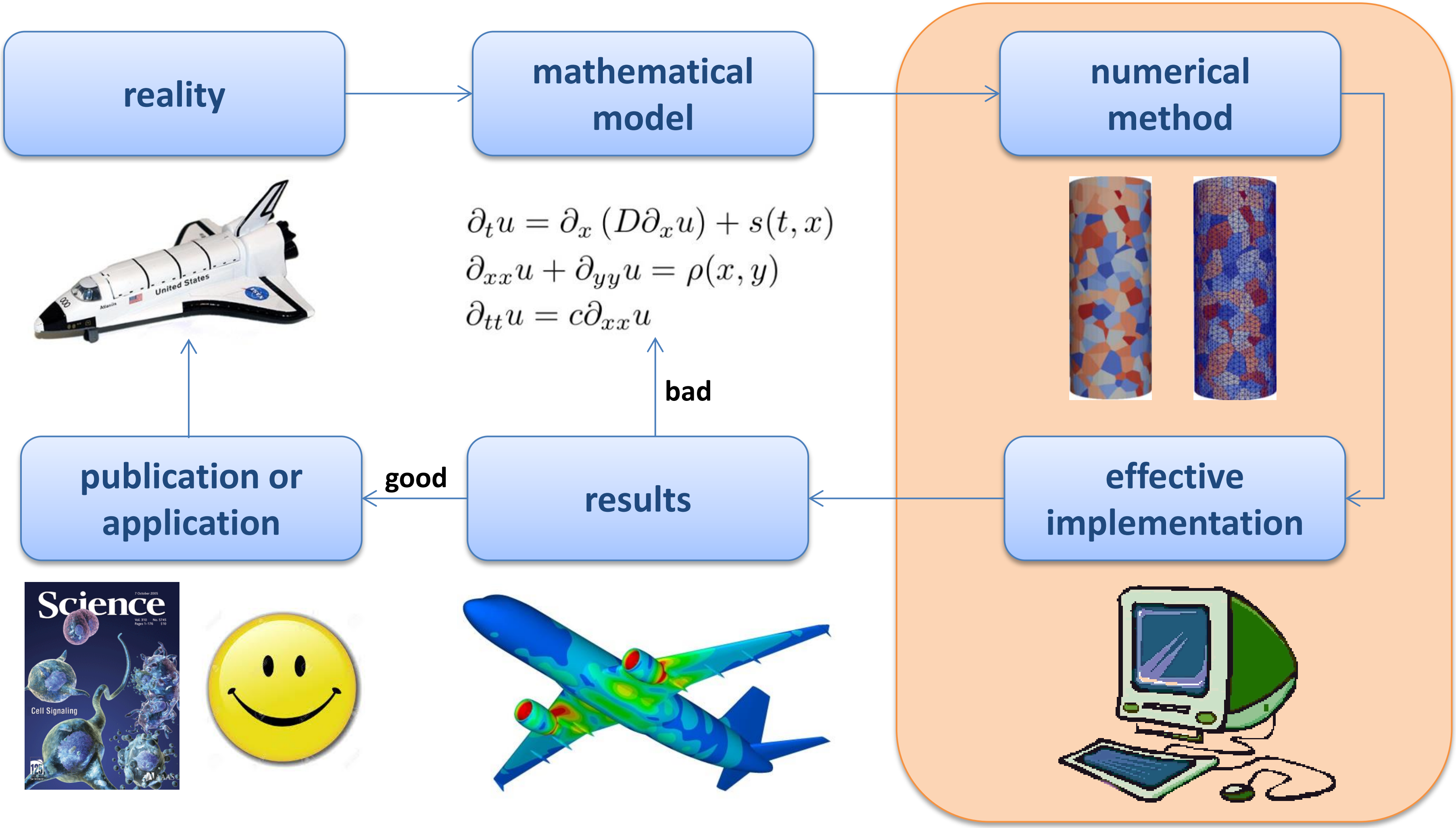
Computational Models in Engineering

How we do what we do…



Energy Minimization

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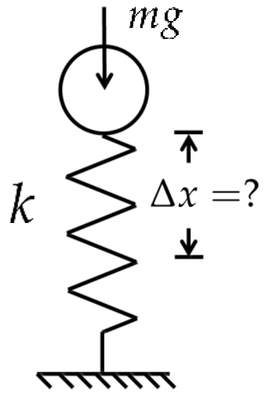
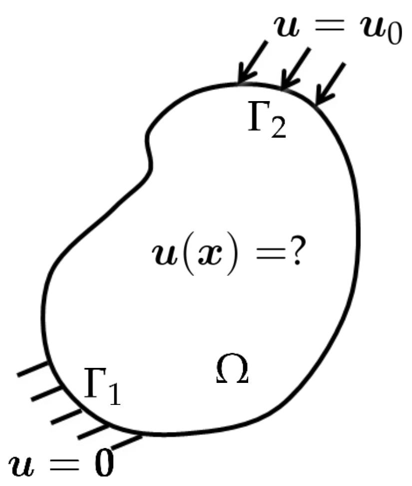
energy minimization of single spring:



- system energy : $\Psi(\Delta x) = -mg\Delta x + \frac{1}{2}k\Delta x^2$
- minimize Ψ : $\frac{\mathrm{d}\Psi}{\mathrm{d}\Delta x} = 0 \quad \Rightarrow \Delta x = \frac{mg}{k}$

solid mechanics example:



- unknown: displacement field: $\boldsymbol{u}(\boldsymbol{x})$
- local stored energy : $W(\nabla \boldsymbol{u}(\boldsymbol{x}))$
- system energy : $\Psi(\boldsymbol{u}(\boldsymbol{x})) = \int_\Omega W(\nabla \boldsymbol{u}(\boldsymbol{x}))\mathrm{d}\,\boldsymbol{v}$
- **our problem:**
  $\boldsymbol{u}(\boldsymbol{x}) = \arg\min \Psi(\boldsymbol{u}(\boldsymbol{x}))$
  subject to: $\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{0}$ on Γ_1, $\quad \boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}_0$ on Γ_2

Finite Element Method

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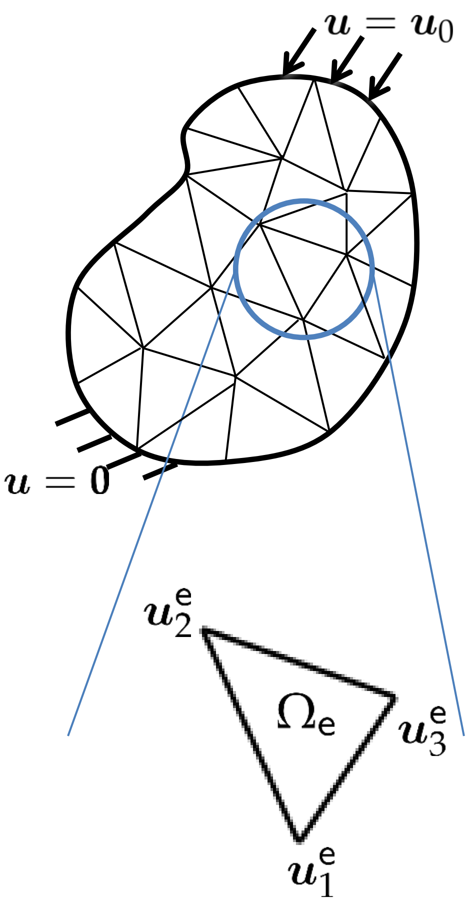
finite element discretization:



FEM idea:

- discretize the domain in space using elements;
- use unknowns on the nodes to approximate the unknown field;
- transform the original variational problem to a **discretized optimization problem**.

- displacement discretization : $\boldsymbol{u}(\boldsymbol{x}) \approx \boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots \boldsymbol{u}_n]^{\mathrm{T}}$
- system energy is the summation from all elements :

$$\Psi(\boldsymbol{u}(\boldsymbol{x})) = \Psi(\boldsymbol{U}) = \sum \int_{\Omega_e} W(\boldsymbol{U}_e) \mathrm{d}\,\boldsymbol{v}$$

- stationary point, force vector : $\boxed{\boldsymbol{F}(\boldsymbol{U}) = \frac{\partial \Psi}{\partial \boldsymbol{U}} = \boldsymbol{0}}$ subject to B.Cs.

system of nonlinear equations.

Finite Element Method

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our problem:

find displacements at each node $\boldsymbol{U}_s = [\boldsymbol{u}_1, \boldsymbol{u}_2, ...\boldsymbol{u}_n]^{\mathrm{T}}$ satisfying $\boldsymbol{F}(\boldsymbol{U}_s) = \frac{\partial \Psi}{\partial \boldsymbol{U}} = \boldsymbol{0}$

numerical root finding via Newton's tangent method:

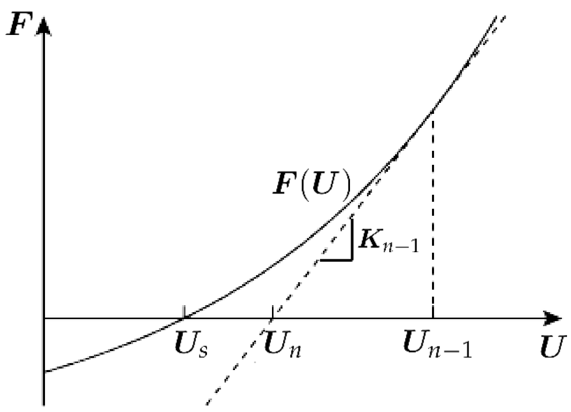
- given initial guess: $\boldsymbol{U}_0$
- do the following updates until $\boldsymbol{F}(\boldsymbol{U}_n) \approx \boldsymbol{0}$

$$\boldsymbol{U}_n = \boldsymbol{U}_{n-1} - \boldsymbol{K}_{n-1}^{-1} \boldsymbol{F}(\boldsymbol{U}_{n-1}), \quad \text{where} \quad \boldsymbol{K} = \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}} = \frac{\partial^2 \Psi}{\partial \boldsymbol{U} \partial \boldsymbol{U}}$$

given displacements at each node $\boldsymbol{U}$, we need to compute:

- system energy: $\Psi(\boldsymbol{U})$
- system force vector: $\boldsymbol{F}(\boldsymbol{U}) = \frac{\partial \Psi}{\partial \boldsymbol{U}}$
- system tangent matrix: $\boldsymbol{K}(\boldsymbol{U}) = \frac{\partial^2 \Psi}{\partial \boldsymbol{U} \partial \boldsymbol{U}}$

Newton's method illustration:



General Finite Element Code Building Structure

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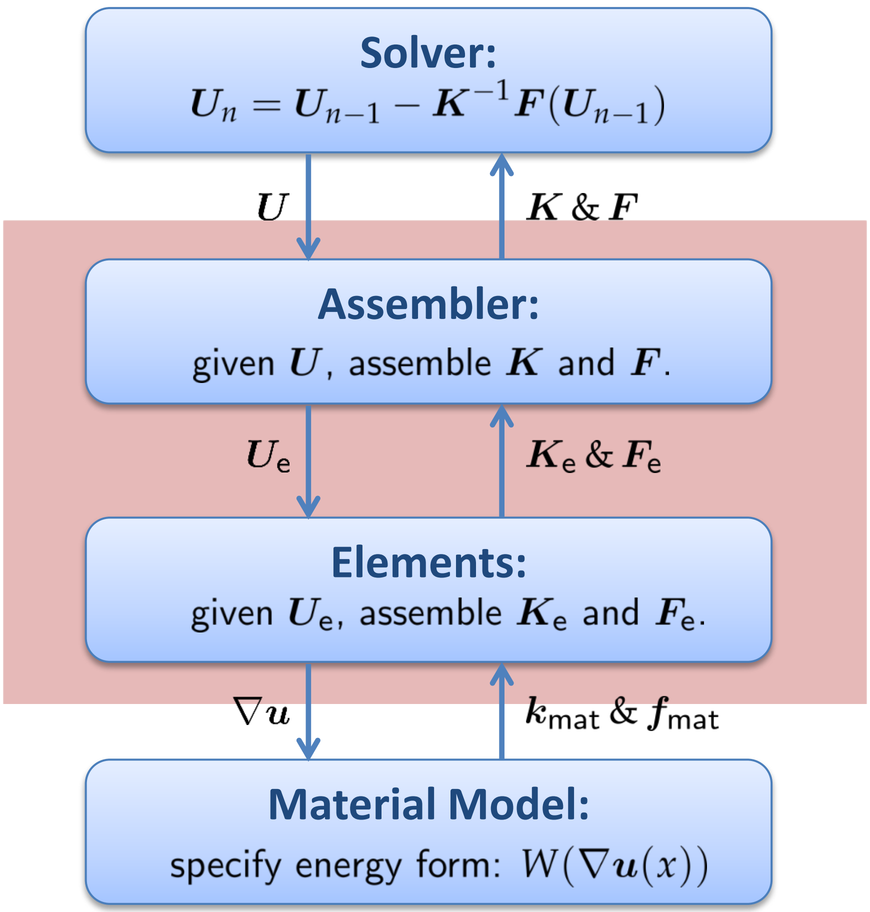
generic finite element code structure:



example:
Newton's method, conjugate gradient, …

example:
triangle, quadrilateral, tetrahedron,. …

example:
elastic, plastic, viscosity, …

Element & Assembler

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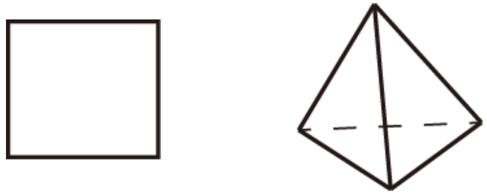
Element class member functions:

```
elementEnergy computeEnergy(dispsAtElementNodes);
elementForces computeForce(dispsAtElementNodes);
elementTangentMatrix computeTangentMatrix(dispsAtElementNodes);
```

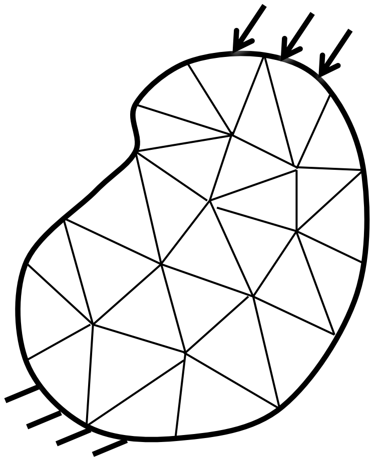
quad and tet elements:



Assembler class member functions:

```
systemEnergy assembleEnergy(dispsAtGlobalNode){
  double energy=0;
  for (eleId=0; ...){
    //get displacements of current element
    energy+=elements[eleId].computeEnergy(eleDisps);
  }
  return energy;
};
systemForces assembleForceVector(dispsAtGlobalNode) {...};
systemTangentMatrix assembleTangentMatrix(dispsAtGlobalNode){...};
```

global system:



Design By Inheritance and Virtual Functions

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VectorXd && MatrixXd:

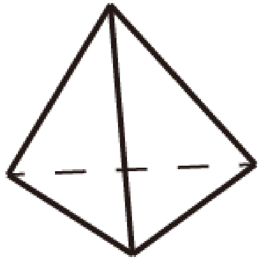
dynamical allocated vector/matrix the size of which is determined at runtime.

element interface:

```
class ElementBase {
public:
  using ElementVector = VectorXd; //used to expression the dimensionality
  using ElementDisplacements = std::vector<ElementVector>; //size of vector = numberOfNodes
  using ElementForce = std::vector<ElementVector>;
  using ElementTangentMatrix = MatrixXd;

  virtual double computeEnergy(const ElementDisplacements&) const = 0;
  virtual ElementForce computeForce(const ElementDisplacements&) const = 0;
  virtual ElementTangentMatrix computeTangentMatrix(const ElementDisplacements&) const = 0;
}
```

tetrahedron element:



specific element implementation:

```
class Tetrahedron : public ElementBase {
public:
  double
  computeEnergy(const ElementBase::ElementDisplacements&) const override {...};

  ElementBase::ElementForce
  computeForce(const ElementBase::ElementDisplacements&) const override {...};

  ElementBase::ElementTangentMatrix
  computeTangentMatrix(const ElementBase::ElementDisplacements&) const override {...};
}
```

Design By Inheritance and Virtual Functions

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California Institute of Technology

assembler class should use pointers to the interface

```
class Assembler {
public:
  using Vector = VectorXd;
  using Displacements = std::vector<Vector>;
  using ForceVector = VectorXd;
  using TangentMatrix = SparseMatrix;

  double assembleEnergy(const Displacements& globalDisplacements) const ;
  ForceVector assembleForceVector(const Displacements& globalDisplacements) const;
  TangenetMatrix assembleTangentMatrix(const Displacements& globalDisplacements) const;

private:
  std::vector<ElementBase*> elements;
}
```

implementation of energy assembler:

```
double
Assembler::assembleEnergy(const Displacements& globalDisplacements) const {
  double energy=0;
  for (auto& element : elements){
    //get displacement for each element (eleDisps)
    energy+=element->computeEnergy(eleDisps);
  }
  return energy;
};
```

Difficulties with Interface

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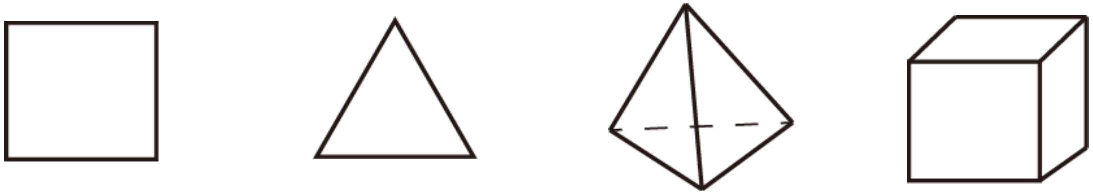
element interface:

```
class ElementBase {
public:
  using ElementVector = VectorXd;
  using ElementDisplacements = std::vector<ElementVector>;
  using ElementForce = std::vector<ElementVector>;
  using ElementTangentMatrix = MatrixXd;

  virtual double computeEnergy(const ElementDisplacements&) const =0;
  virtual ElementForce computeForce(const ElementDisplacements&) const =0;
  virtual ElementTangentMatrix computeTangentMatrix(const ElementDisplacements&) const =0;
}
```

different elements have different properties:



problems:

- interface cannot express information about specific properties of each element type (e.g. number of nodes, dimension, etc.)
- checking preconditions incurs heavy run time cost.

Implementation and Performance

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assembler class containing pointers leads to …

- **choice of pointer:** `std::unique_ptr`, `std::shared_ptr`, raw pointer?
- **more implementation and maintaining work:**
  - copy constructor: `Assembler(const Assembler&);`
  - copy assignment operator: `Assembler& operator=(const Assembler&);`
  - move constructor: `Assembler(Assembler&&) noexcept;`
  - move assignment operator: `Assembler& operator=(Assembler&&) noexcept;`
  - destructor: `~Assembler();`
  - virtual constructor: `Tetrahedron* clone();`

performance problem:

- an extra v-pointer in every inherited class (large data type: typically 8 bytes);
- every function call involves pointer tracing (cache unfriendly);
- harmful to data alignment;
- impossible for function inlining.

(a performance study available at *https://github.com/yingryic/performance_study/*)

Template Alternative (our approach)

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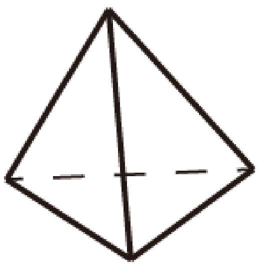
`Matrix<double, NumberOfRows, NummberOfCols>`:

statically allocated matrix whose size should be known at compile time.

tetrahedron element:



element classes are not derived from any class:

```
class Tetrahedron {
public:
  const static int NumberOfNodes = 4;
  const static int SpatialDimension = 3;
  const static int NumberOfDofs = NumberOfNodes*SpatialDimension;

  using ElementVector = Matrix<double, SpatialDimension, 1>;
  using ElementDisplacements = std::array<ElementVector, NumberOfNodes>;
  using ElementForce = std::array<ElementVector, NumberOfNodes>;
  using ElementTangentMatrix = Matrix<double, NumberOfDofs, NumberOfDofs>;

public:
  double
  computeEnergy(const ElementDisplacements& elementDispls) const {...};
  ElementForce
  computeForce(const ElementDisplacements& elementDispls) const {...};
  ElementTangentMatrix
  computeTangentMatrix(const ElementDisplacements& elementDispls) const {...};
};
```

Template Alternative (our approach)

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assembler class contains element objects rather than pointers:

```
template<class ElementType>
class Assembler {
public:
  static const int SpatialDimension = ElementType::SpatialDimension;
  using ElementVector = typename ElementType::ElementVector;
  using ElementDisplacements = typename ElementType::ElementDisplacements;
  using Displacements = std::vector<ElementVector>;
  using ForceVector = VectorXd;

  double assembleEnergy(const Displacements& displs) const {
    double energy=0;
    for (auto& element : elements){
      ElementDisplacement eleDisps=...;
      energy += element.computeEnergy(eleDisps);
    }
    return energy;
  };

  ForceVector assemblerForceVector(const Displacements& displs) const {...};
  SparseMatrix assembleTangentMatrix(const Displacements&displs) const {...};

private:
  std::vector<ElementType> elements;
  ... ...
};
```

Template vs. Virtual Functions

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advantage of using template:

- dimensionality mismatch can be caught at compile time.
- no extra v-pointer and virtual function calls.
- can rely on the default copy/move constructor/assignment operator, destructor, etc.
- possible for function inlining (compiler can see the implementation).

advice from *Bjarne Stroustrup*:

- Prefer a template over derived classes when run-time efficiency is at a premium.
- Prefer derived classes over a template if adding new variants without recompilation is important.
- Prefer a template over derived classes when no common base can be defined.
- Prefer a template over derived classes when built-in types and structures with compatibility constraints are important.

The C++ Programming Language, 3rd Edition, chapter 13.8

Performance Concerns

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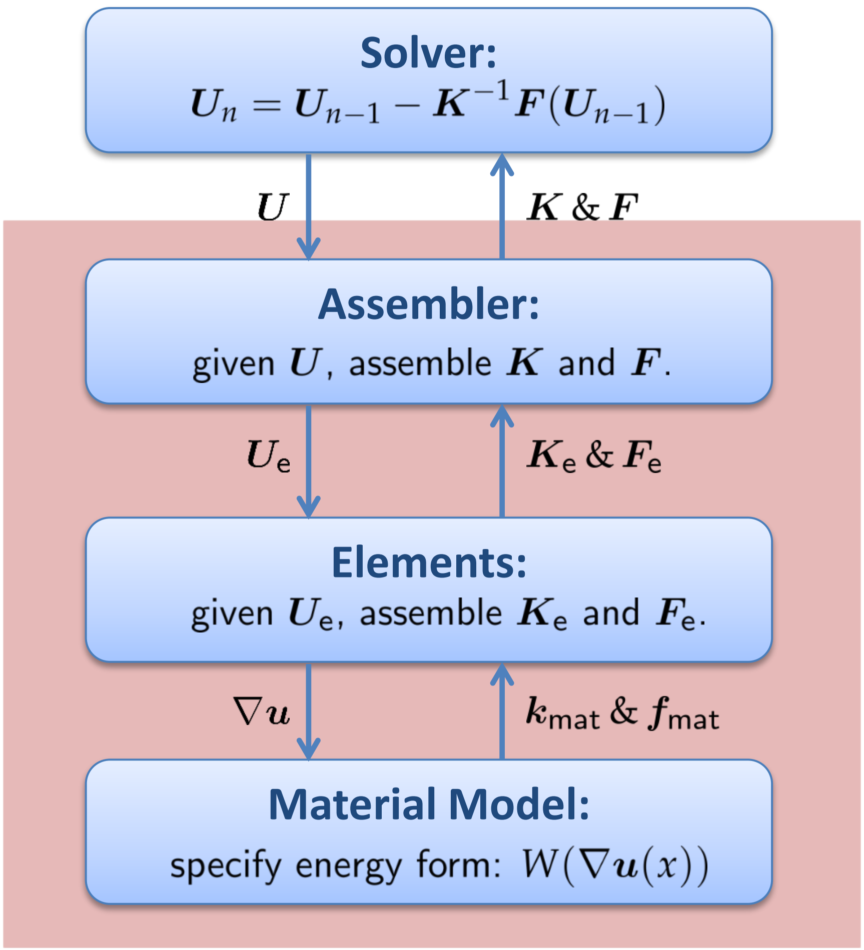
generic finite element code structure:



computation bottle neck:

- **solver level**: time complexity O(n^3); finding solution to system of linear equations
- **assembler level**: time complexity O(n); usually involves complex underlying material models

concurrency techniques:

- **solver level**:
- utilize threaded linear algebra libraries (ViennaCL, Intel Math Kernal Library)
- **threaded assembler.**
- assembleEnergy;
- assembleForceVector;
- assembleTangentMatrix;

Case Study of Threaded Assembler

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California Institute of Technology

experimental setup:

- parallelize assembly of 681,942 tetrahedron elements in a pillar compression example
- time performance with different number of threads

hardware and system configuration:

- cpu: Intel Xeon E5-2680 CPU, 8 cores;
- memory: 24GB;
- system: Redhat 64 bit;
- compile: g++-4.8.

threading library: openmp

finite element discretization of pillar compression test:

Assemble Energy

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single thread Energy Assembler (pseudo code):

```
initialize globalEnergy=0

#pragma omp parallel for reduction (+:globalEnergy)
for each element:
  get element displacements and node Id
  compute elementEnergy
  add elementEnergy to globalEnergy

return globalEnergy
```

multithread Energy Assembler (pseudo code):

```
initialize globalEnergy=0
#pragma omp parallel {
  initialize threadLocalEnergy=0
#pragma omp for
  for each element {
    get element displacements and node Id
    compute elementEnergy
    add elementEnergy to threadLocalEnergy
  }
#pragma omp critical
  globalEnergy+=threadLocalEnergy
}
return globalEnergy
```

run time of assemble energy with different numbers of threads:

#. of threads	run time (s)	speedup
1	0.1588	1.00
2	0.0805	1.97
3	0.0561	2.83
4	0.0474	3.35
5	0.0378	4.20
6	0.0324	4.90
7	0.0285	5.56
8	0.0251	6.33

Assemble Force Vector

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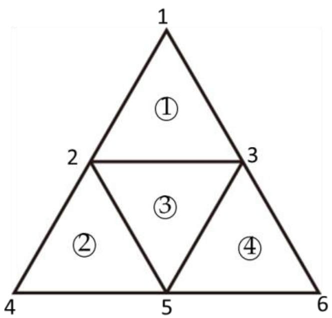
system with four elements:



problem dimension: 2;
degree of freedom: 1

$$\boldsymbol{U} : 6 \times 1$$

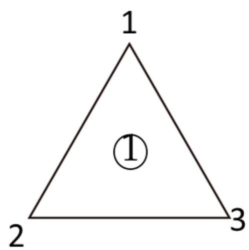
$$\boldsymbol{F} : 6 \times 1$$

$$\boldsymbol{K} : 6 \times 6$$

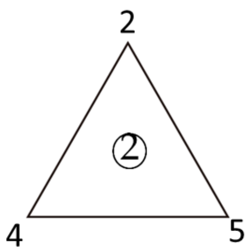
final force vector:

$$\boldsymbol{F} = \begin{bmatrix} F_1^1 \\ F_2^1 + F_1^2 + F_3^3 \\ F_3^1 + F_2^3 + F_1^4 \\ F_2^2 \\ F_3^2 + F_1^3 + F_2^4 \\ F_6^4 \end{bmatrix}$$

assemble force in action:



$$\boldsymbol{F}_{\mathrm{e}}^1 = \begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{bmatrix} F_1^1 & F_2^1 & F_3^1 \end{bmatrix} \end{array} \xrightarrow{\text{assemble}} \boldsymbol{F} = \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} F_1^1 & F_2^1 & F_3^1 & . & . & . \end{bmatrix} \end{array}$$



$$\boldsymbol{F}_{\mathrm{e}}^2 = \begin{array}{c} \begin{array}{ccc} 2 & 4 & 5 \end{array} \\ \begin{bmatrix} F_1^2 & F_2^2 & F_3^2 \end{bmatrix} \end{array} \xrightarrow{\text{assemble}} \boldsymbol{F} = \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} F_1^1 & F_2^1 + F_1^2 & F_3^1 & F_2^2 & F_3^2 & . \end{bmatrix} \end{array}$$

source of data race: nodes shared by different elements will be modified by different elements.

Assemble Force Vector (Solution #1)

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single thread Force Assembler (pseudo code):

```
initialize globalForceVector=0

for each element:
  get element displacements and node Id
  compute elementForce
  add elementForce to globalForceVector

return globalForceVector
```

multithread Force Assembler (pseudo code):

```
initialize globalForceVector=0
#pragma omp parallel {
  initialize a threadLocalForceVector=0
#pragma omp for
  for each element {
    get element displacements and node Id
    compute elementForce
    add elementForce to threadLocalForceVector
  }
#pragma omp critical
  globalForceVector+=threadLocalForceVector
}
return globalForceVector
```

serialized adding vectors may harm performance.

run time of assemble force vector with different numbers of threads:

#. of threads	run time (s)	speedup
1	0.2598	1.00
2	0.1350	1.93
3	0.1033	2.52
4	0.0785	3.32
5	0.0670	3.89
6	0.0569	4.57
7	0.0515	5.05
8	0.0462	5.63

Assemble Force Vector (Solution #2)

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key idea: each thread writes to the designated position directly.

avoiding data race:

- prepare a number of locks, each lock protects certain nodes;
- when adding entries: lock the corresponding lock, update entry, then release the lock.

multithread Force Assembler (lock version):

```
initialize globalForceVector=0
parallel prepare n locks
#pragma omp parallel for {
  for each element {
    get element displacements and node Id
    compute elementForce
    for each node
      calculate lock id
      set corresponding lock
      add elementForce to globalForceVector
      unset lock
  }
}
return globalForceVector
```

each lock protects 10 nodes:

#. of threads	run time (s)	speedup
1	0.3065	1.00
2	0.1573	1.95
4	0.0979	3.13
6	0.0608	5.05
8	0.0452	6.79

each lock protects 1000 nodes:

#. of threads	run time (s)	speedup
1	0.3022	1.00
2	0.1626	1.86
4	0.1019	2.97
6	0.0801	3.77
8	0.0731	4.13

Assemble Tangent Matrix

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function definition:

```
SparseMatrix assembleTangentMatrix(const Displacements&) const;
```

difficulties when working with sparse matrices:

- only stores nonzero elements;
- inserting new elements would involve linear time copying;
- usually constructing sparse matrix from *triplets* (linear time w.r.t the size of the triplets).

single thread matrix assembler (pseudo code):

```
//estimate #. nonzero entries (e.g. sparse level 1%)
initialize a global triplets
part 1:
for each element:
  get element displacements and node Id
  compute element tangent matrix
  figure out indices in the sparse matrix
  push indices and nonzero value into global triplets
part 2:
construct sparse matrix from the global triplets

return sparse matrix
```

sample run time in different parts:

part 1: 3.00s
part 2: 2.283s

parallelizing both parts is necessary.

Part2: Build Sparse Matrix from Triplets

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overall speedup factors when comparing to MATLAB:

Data Set Hardware	MATLAB Time	Serial Time	Serial Speedup	Parallel Time	Parallel Speedup
1 on C1	3.52	1.51	2.33×	0.65	5.39×
2 on C1	3.74	1.87	2.00×	0.83	4.42×
3 on C1	3.49	1.67	2.09×	0.76	4.55×
1 on C2	3.49	1.61	2.17×	0.33	10.2×
2 on C2	4.39	2.95	1.49×	0.46	9.71×
3 on C2	3.46	1.78	1.96×	0.43	9.01×

C1: 6 cores; C2: 16 cores.

references:

Fast MATLAB compatible sparse assembly on multicore computers, *Stefan Engblom and Dimtar Lukarski*

run time of parallel building sparse matrix from triplets:

#. of threads	run time (s)	speedup
1	2.282	1.00
2	1.148	1.99
3	0.799	2.86
4	0.627	3.64
5	0.506	4.50
6	0.438	5.21
7	0.389	5.86
8	0.353	6.46

Part1: Parallel Building of Triplets (Solution #1)

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similar idea as assemble energy:

- each thread writes to its local triplets list;
- once thread finishes its work, lock global triplets, pushes local triplet list into global triplets.

multithread Matrix Assembler (pseudo code):

```
initialize globalTriplets
#pragma omp parallel {
  initialize localTriplets
#pragma omp for
  for each element:
    get element displacements and node Id
    compute element tangent matrix
    figure out indices in the sparse matrix
    push indices and nonzero value into localTriplets
#pragma omp critial
  push localTriplets into global triplets
}
```

serialized copying worsens scaling

run time of parallel building triplets:

#. of threads	run time (s)	speedup
1	3.862	1.00
2	2.650	1.46
3	2.542	1.52
4	1.969	1.96
5	2.130	1.81
6	2.175	1.78
7	1.942	1.99
8	1.711	2.26

Part1: Parallel Building of Triplets (Solution #2)

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idea:

- parallelize the gathering of copies of triplets from each thread into a vector of triplets;
- get the total number of entries by summing the size of the triplets from the gathered vector;
- initialize global triplets with right number of entries
- parallel copy each of the local triplets into the right position

multithread Matrix Assembler (pseudo code):

```
initialize threadTripletsVector(numberOfThreads);
#pragma omp parallel {
  initialize localTriplets
#pragma omp for
  for each element:
    get element displacements and node Id
    compute element tangent matrix
    figure out indices in the sparse matrix
    push indices and nonzero value into localTriplets
#pragma omp critial
  threadTripletsVector.push_back(std::move(localTriplets))
}
compute total number of entries and initialize globalTriplets
#pragma omp parallel{
   ith thread copy the ith threadTriplets into globalTriplets
}
```

run time of parallel building of triplets:

#. of threads	run time (s)	speedup
1	3.329	1.00
2	1.754	1.89
3	1.293	2.57
4	1.072	3.11
5	0.902	3.69
6	0.801	4.15
7	0.730	4.56
8	0.666	5.00

Overall Performance of Assemble Tangent Matrix

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#. of threads	run time(s)	speedup
1	5.598	1.00
2	2.890	1.94
3	2.087	2.68
4	1.697	3.30
5	1.390	4.02
6	1.255	4.46
7	1.127	4.97
8	1.012	5.53

Summary & Conclusion

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Template & Inheritance

- Designing finite element library by **templates** and **static programming techniques** could lead better performing, maintainable and safer code.
- Consider using template over inheritance (virtual function) approach unless constraints on recompilation time and size of executables are crucial.

Performance

- Threading both **solver** and **assembler** are necessary to utilize **multi core machine** to build scalable program.
- **Critical sessions** should be used **with caution** in order to reach better scalability. General guide line would be only allow **constant time operations** in critical sessions.

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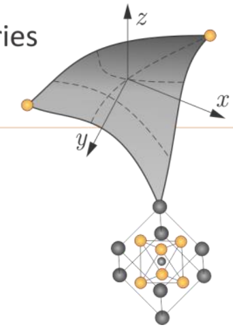

Thank you for your interest!

Questions & Comments

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