



Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich



Scalable Multi-level Preconditioners for Variable Viscosity Stokes Flow Problems Arising from Geodynamics

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Geodynamics := ???



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Outline

- Geodynamic background and motivations
- Spatial discretisations for long term geodynamic applications
- Newton formulation
- Scalable preconditioners for Saddle point problems
- Two-dimensional geodynamic examples
- Geometric multi-grid with matrix-free smoothers
- Three-dimensional geodynamic applications

Convective Engine of the Earth



http://dreamtigers.wordpress.com/2011/05/11/plate-tectonic-metaphor-illustrations-cmu/





- Long time scale process. Very viscous, creeping flow regime
- Highly temperature dependent viscosity large contrast in material properties (lel0)
- Stokes like Rayleigh-Bénard convection with strongly variable viscosity

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Regional Geodynamics Processes



- Topography variations
- Large variation in length scales
- Presence of faults (material failure)
- Melting

- Complex constitutive behaviour
- Large deformation
- Deformation past the onset of material failure

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Coupled Regional / Global Processes





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Coupled Regional / Global Processes



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Coupled Regional / Global Processes



nttp://en.wikipedia.org/wiki/File:Oceanic_spreading.svg

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Geology is Complex

Zagros Mountains



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Geology is Complex

- **European Alps** (Kissling, 2012) European plate East Alpine slab Adriatic plate Apennine
- Inherently 3D
- Discontinuous properties
- Severe ductile folding + faulting
- Small length scales
 - "...a total mess" even by geological standards



Geodynamic Motivations Continental rifting



- Follow the **4D** evolution of rocks over 60millions year time spans \longrightarrow large deformation
- Complex constitutive laws
- Large contrast in material properties
- Deformation past the onset of material failure

Problem Statement

• Incompressible, Variable Viscosity (VV) Stokes:

$$\begin{bmatrix} 2\eta D_{ij}(\boldsymbol{u}) \end{bmatrix}_{,j} - p_{,i} = f_i \quad \text{in } \Omega$$
$$u_{k,k} = 0$$
$$u_i = \bar{u}_i \quad \text{on } \Gamma_D$$
$$\boldsymbol{\sigma}_{ij}n_j = \bar{t}_i \quad \text{on } \Gamma_N$$

- Non-linear constitutive behaviour
- Evolution of coefficients

$$\frac{D\eta}{Dt} = 0, \qquad \frac{Df_i}{Dt} = 0$$

• Non-linear boundary conditions

• Conservation of Energy:
$$\frac{DT}{Dt} = [\kappa T_{,k}]_{,k} + Q$$

Problem Statement: Coefficients

Incompressible, Variable Viscosity (VV) Stokes:

$$\begin{bmatrix} 2\eta D_{ij}(\boldsymbol{u}) \end{bmatrix}_{,j} - p_{,i} = f_i \quad \text{in } \Omega$$
$$u_{k,k} = 0$$

• Non-linear constitutive behaviour $~(\eta)$

Arrhenius [u,p,T dependence]

$$\eta = A(\sqrt{I'_2})^{\alpha} \exp\left(\frac{E+Vp}{nRT}\right) \qquad I'_2 = \frac{1}{2}D_{ij}D_{ij}$$

Plasticity [u,p dependence]

$$\begin{split} F_s &:= \sqrt{J'_2} - \tau_{\text{yield}}^{VM}, \quad \text{where } \tau_{\text{yield}}^{VM} := \text{const.} \quad J'_2 = \frac{1}{2} \tau_{ij} \tau_{ij} \\ F_s &:= \sqrt{J'_2} - \tau_{\text{yield}}^{DP}, \quad \text{where } \tau_{\text{yield}}^{DP} := C_0 \cos(\phi) + p \sin(\phi), \\ \eta &= \frac{\tau_{\text{yield}}}{2\sqrt{I'_2}} \quad \text{if } \sqrt{J'_2} > \tau_{\text{yield}}, \end{split}$$

• Boussinesq approximation (f_i)





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Problem Statement

Incompressible, Variable Viscosity (VV) Stokes:

 $\begin{bmatrix} 2\eta D_{ij}(\boldsymbol{u}) \end{bmatrix}_{,j} - p_{,i} = f_i \quad \text{in } \Omega$ $u_{k,k} = 0 \quad u_i = \bar{u}_i \quad \text{on } \Gamma_D$ $\sigma_{ij}n_j = \bar{t}_i \quad \text{on } \Gamma_N$



- Non-linear constitutive behaviour
- Evolution of coefficients

$$\frac{D\eta}{Dt} = 0, \qquad \frac{Df_i}{Dt} = 0$$

Use independent spatial discretisations for (i) the flow variables (velocity, pressure) \longrightarrow Mixed FEM [Q2-P1] (ii) coefficients (viscosity, density) \longrightarrow Lagrangian markers

(aka Material Point Method)

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Spatial Discretisation (FE)

Discrete Variational Problem (with interpolated coefficients) Seek $(\boldsymbol{u}_h, p_h) \in \boldsymbol{V}^h \times Q^h$ with $\eta^\lambda \in X$ and $\boldsymbol{f}^\lambda \in (X)^d$ such that $A(\boldsymbol{u}_h, \boldsymbol{v}_h) + B(\boldsymbol{v}_h, p_h) = F(\boldsymbol{v}_h)$ $B(\boldsymbol{u}_h, q_h) = 0$ for all $(\boldsymbol{v}_h, q_h) \in \boldsymbol{V}_0^h \times Q^h$. $A(\boldsymbol{u}, \boldsymbol{v}) = \int_{\Omega} \sum_{i,j=1}^d 2\eta^\lambda D_{ij}(\boldsymbol{u}) D_{ij}(\boldsymbol{v}) \, dV,$ $B(\boldsymbol{v}, q) = \int_{\Omega} q\nabla \cdot \boldsymbol{v} \, dV,$ $F(\boldsymbol{v}) = \int_{\Omega} \boldsymbol{v} \cdot \boldsymbol{f}^\lambda \, dV + \int_{\Gamma_N} \boldsymbol{v} \cdot \bar{\boldsymbol{t}} \, dS.$ $V := (V)^d = \left\{ \boldsymbol{v} \in (H^1(\Omega))^d \, | \, \boldsymbol{v} = \bar{\boldsymbol{u}} \text{ on } \Gamma_D \right\},$ $Q := \left\{ q \in L_2(\Omega) : \int_{\Omega} q \, dV = 0 \right\},$ $X := \left\{ x \in L_2(\Omega) \right\},$

 Reconstruct coefficients (viscosity, density) for the flow problem using material points

Spatial Discretisation (MPM)

 Reconstruct coefficients (viscosity, density) at quadrature points for the flow problem using material points



Particle In Cell (PIC) Harlow & Welch, Phys. Fluids, (1965)

Material Point Method (MPM) Sulsky & Brackbill, JCP, (1991)

$$A(\boldsymbol{u}, \boldsymbol{v}) = \int_{\Omega} \sum_{i,j=1}^{d} 2\eta^{\lambda} D_{ij}(\boldsymbol{u}) D_{ij}(\boldsymbol{v}) \, dV,$$
$$F(\boldsymbol{v}) = \int_{\Omega} \boldsymbol{v} \cdot \boldsymbol{f}^{\lambda} \, dV + \int_{\Gamma_N} \boldsymbol{v} \cdot \bar{\boldsymbol{t}} \, dS.$$

[a] Local L2 projection (Q1)



[b] Piecewise constant (PO)







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Newton Framework

STOKES NON-LINEAR RESIDUALS

$$\hat{F}_{u_i} := \left[2\eta(\boldsymbol{u}, p) D_{ij}(\boldsymbol{u}) \right]_{,j} - p_{,i} - f_i(\boldsymbol{u}, p)$$
$$\hat{F}_c := u_{k,k}$$

DISCRETISE

$$F_u = Au - Bp - f$$
$$F_c = B^T u$$

LINEARISE

$$\begin{bmatrix} A + \delta A & B + \delta B \\ B^T + \delta B^T & 0 \end{bmatrix} \begin{bmatrix} \delta u \\ \delta p \end{bmatrix} = - \begin{bmatrix} F_u \\ F_c \end{bmatrix}$$

STOKES JACOBIAN

$$\mathcal{J}_s = \begin{bmatrix} A + \delta A & B + \delta B \\ B^T + \delta B^T & 0 \end{bmatrix}$$



void FormFunction(Vec X,void *ctx) {

- Extract u,p from X
- Update nonlinearities on markers $f:=\tau_{II}-\tau_y\leq 0$

$$\tau_{II} := \sqrt{\frac{1}{2}\tau_{ij}\tau_{ij}}$$
$$\eta_{vp} = \begin{cases} \frac{\tau_y}{\sqrt{2\epsilon_{ij}\epsilon_{ij}}} & \text{if } \tau_{II} > \tau_y \\ \eta & \text{otherwise} \end{cases}$$

- Project marker properties to QP
- Evaluate FE Stokes residuals

$$F_u^e = A^e u^e - Bp^e - f^e$$
$$F_c^e = (B^e)^T u^e$$

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Saddle Point Preconditioners

Newton update requires linear solve



$$\mathcal{A} = \begin{bmatrix} A + \delta A & B + \delta B \\ B^T + \delta B^T & 0 \end{bmatrix}$$
$$x = \begin{bmatrix} \delta u \\ \delta p \end{bmatrix} \qquad b = - \begin{bmatrix} F_u \\ F_c \end{bmatrix}$$

The ideal approach should be optimal in the sense that the convergence rate of method will be bounded independently of:

- the discretisation parameters (e.g. grid resolution)
- the constitutive parameters (e.g. smooth vs. discontinuous viscosity)
- the constitutive behaviour (e.g. isotropic vs. anisotropic)
- and we desire that the solution is obtained in O(n) time... i.e. multigrid

These are a challenging set of requirements



Viscosity contrasts

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Newton MG for Saddle Point Systems

Apply a Krylov method (e.g. FGMRES, GCR) directly to

$$\mathcal{A}x = b$$

right preconditioned with

$$\mathcal{B}_{s} = \begin{bmatrix} A' & B\\ 0 & -S^{*} \end{bmatrix} \quad \text{where} \quad S^{*} = \int_{\Omega_{e}} \frac{1}{\bar{\eta}_{e}} M_{i} M_{j} \, dV$$
$$S^{*} \approx S = B^{T} A^{-1} B$$

Standard upper block triangular preconditioner, demonstrated to be effective for VV Stokes

- See Elman's book (2005)
- Burstedde, CMAME, (2009)
- Geenen et al, G3, (2009) Grinevich & Olshanskii, SIAM J. Comput, (2009)



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Applying the action of the Stokes preconditioner on a vector t

$$s = \mathcal{B}_s^{-1}t$$

requires the action of

$$u = A'^{-1}v \quad \longrightarrow \quad$$

Apply Algebraic MultiGrid (AMG) or Geometric MultiGrid (GMG) to **A'**

Two-dimensional Examples

Prototype geodynamic processes

Crustal/lithospheric Problem (Boundary driven processes)



Upper Mantle Problem (Body force driven processes) Topography dense rigid plate weak less dense material Length scale 100-1000 km Reverted density gradient, thick low viscosity layer

weak density contrasts, gravitationally stable (density increases with depth) thick high viscosity layer.

Numerical realisations



[May, Le Pourhiet, JCP, In prep.]

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Visco-plastic Shortening







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Visco-plastic Shortening



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Subduction: Coordinate Evolution



Subduction: Coordinate Evolution



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Subduction: Coordinate Evolution



Moving to 3D: pTatin3d

["p" stands for PETSc, pragmatic and pedantic]

- Open source project with the following features
 - Fully parallel (flat MPI), robust and scalable 3D FE-MPM discretisation and solvers for non-linear variable viscosity Stokes
 - Physics is extensible
 - Flexible solver design (defer as many choices as possible to run time)
 - Low memory to maximize numerical resolution, maximize resources and permit wide usability to geodynamic community without massive HPC access
 - Employ algorithms which exploit modern multi-core architectures. Target hardware; IBM BG/Q, Cray XE6

Parallel algebra support provided by PETSc (<u>www.mcs.anl.gov/petsc</u>)



Performance Issues

"Strong" smoothers require assembling operators (e.g. CG/ICC - GMRES/ILU)

STORAGE IS EXPENSIVE

- + temporary vectors for the solver
- (Q2) 64 x 64 x 64 ~ 19.3 GB + whatever else you might need... 3 x **A***ii*: (Q2) 64 x 64 x 64 ~ 6.4 GB
 - e.g. markers, quadrature point fields...



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A:

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 - + whatever else you might need...
 - e.g. markers, quadrature point fields...



"ulysse": [SGI Altix UV 100] 6 nodes; 8 x Xeon E7-8837 (2.67GHz); 8 GB RAM/core

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Performance of

Matrix-Free (MF) SpMV [weak scaling]

"hexagon": [Cray XE6] 696 nodes; 2x16 AMD Interlagos (2.3GHz); 1 GB RAM/core





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Performance of MF-SpMV [strong scaling]

"hexagon": [Cray XE6] 696 nodes; 2x16 AMD Interlagos (2.3GHz); 1 GB RAM/core



Excellent strong scaling when using more than 8 Q2 elements per core

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Convergence History: Stokes



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Single CPU test



* 32 x 32 x 32 : 4 MG levels

- * Single iteration of Stokes solve
- * A u = v terminated when initial residual reduced by 1e6
- * Smoother: Chebychev/Jacobi 6 iterations
- * Coarse grid: LU



Single CPU test



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- * Smoother: Chebychev/Jacobi 6 iterations
- * Coarse grid: LU

Ċ	Coarse level configuration	$\Delta \eta = 10^0$	$\Delta \eta = 10^2$	$\Delta \eta = 10^6$	$\Delta \eta = 10^{10}$	Mem. (GB)
coarse	A, M, M, M	51 (#5)	123 (#13)	532 (#60)	1605 (#179)	0.7
	G, A, M, M	51 (#5)	114 (#12)	185 (#20)	185 (#20)	0.8
	G, G, A, M	51 (#5)	87 (#9)	120 (#13)	130 (#14)	1.2
	G, G, G, A	43 (#5)	51 (#6)	73 (#9)	80 (#10)	4.4

Solve time (sec) (#number of iterations)

G = Galerkin : **A** = Assembled : **M** = Matrix-free

Single CPU test



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- * A u = v terminated when initial residual reduced by 1e6
- * Smoother: Chebychev/Jacobi 6 iterations
- * Coarse grid: LU

Coarse level Mem. $\Delta \eta = 10^{10}$ $\Delta \eta = 10^0$ $\Delta \eta = 10^2$ $\Delta \eta = 10^6$ configuration **(GB)** A, M, M, M 51 (#5) 123 (#13) 532 (#60) 1605 (#179) 0.7 coarse G, A, M, M 185 (#20) 0.8 114 (#12) 185 (#20) 51 (#5) G, G, A, M 120 (#13) 130 (#14) 1.2 51 (#5) 87 (#9) 80 (#10) 73 (#9) G, G, G, A 43 (#5) 51 (#6) 4.4 G = Galerkin : A = Assembled : M = Matrix-free

Solve time (sec) (#number of iterations)

- G Galerkin : A Assembled : M Matrix-free
- Significant gains obtained from using "strong" coarse grid operators memory increase is minimal
- Assembled Galerkin is 38% faster HOWEVER uses 3.7 times more memory

Convergence History: Viscous Block





• Sedimenting sphere

- 32³ elements
- •4 levels
- Coarse Galerkin
- Cheby(4) + Jacobi smoother
- LU coarse

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Parallel Performance

Cores	64	512	4096
Event			
MGSmooth Coarse	1.5907e + 02	2.9855e+01	8.8030e+00
$MatSolve^*$	8.6882e + 01	$1.8791e{+}01$	3.4849e + 00
MGSmooth Fine	5.4153e + 02	$6.8653e{+}01$	9.1118e + 00
MatMult*	8.5636e + 02	1.1249e + 02	1.6264e + 01
$VecDot^*$	4.8386e + 00	1.1783e+00	1.3234e + 00
VecMDot	2.0199e+00	3.8708e-01	2.0188e-01
$VecNorm^*$	1.1429e + 01	2.5994e + 00	4.4239e-01
KSPGMRESOrthog	7.9125e + 00	1.5767e + 00	1.5306e + 00
KSPSolve	9.6860e+02	1.2980e+02	2.1507e+01
J KSP #	24	24	23
A KSP #	100	101	98
MGC oarse KSP $\#$	347	399	495



• Sedimenting sphere

$$R = 0.25$$
$$\Delta \eta = 10^4$$

- 96³ elements
- 3 levels
- Cheby(10) + Jacobi smoother
- $\delta_A^{
 m rel} = 10^{-2}$ Krylov coarse grid solver

Excellent strong scaling. 70% efficiency from 64 to 4096 cores

 $\delta_I^{\rm rel} = 10^{-5}$

 $\delta_{A_C}^{\rm rel} = 10^{-2}$

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Oblique Rifting

in collaboration with L. Le Pourhiet (UPMC, Paris)

Major oil reservoirs have been discovered within the last 10 years in the Equatorial Atlantic. These oil fields were not explored before as companies had classified such "oblique continental margins" as having very low oil potential - an assumption which was largely based on *state-of-the-art 2D modeling*.



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Major oil reservoirs have been discovered within the last 10 years in the Equatorial Atlantic. These oil fields were not explored before as companies had classified such "oblique continental margins" as having very low oil potential - an assumption which was largely based on state-of-the-art 2D modeling.

Strike slip systems in oblique settings have not been selfconsistently modelled before.

3D modelling of continental rifting and break-up is numerically challenging as it requires;

- large domains, 4000 km x 4000 km x 300 km
- simulations to be performed over large time spans, > 30 million years
- resolving the influence of strongly non-linear material behaviour and large viscosity contrasts (1e6) between thin layers (< 10 km)



exist



Oblique Continental Margins

Oceanic crust Thin continental crust **Uplifiting Area Subsiding Area**

One branch is



Non-linear, Arrhenius + Drucker Prager rheology (brittle / ductile)



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model with no shortening develops oblique rifting branches, self consistently. The timing when obliquity occurs may help constrain boundary conditions.

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Vz = 5 mm/yr





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necessary to valid models from field geology Efficient Solution of Nonlinear PDEs - Lyon

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* 128 x 64 x 128 Q2 elements, 20 Myr (1800 time steps, full non-linear solve) 64 cores with ~I GB/core in ~II days

* Same model runs on 18 hours on 1024 cores [Cray XE6] due to good strong scaling capabilities At lower resolution, the asymmetry of propagation, the small faults cutting the oblique margin are not resolved. Such structures are necessary to valid models from field geology

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Rifting at Scale

- Geometry aspect ratio: 12 x 1.5 x 6
- Three level MG hierarchy
 - Viscosity gradients largest in y (coarsening less frequently)
 - Coarsen aggressively in directions with high aspect ratio
- Use Chebyshev + Jacobi smoothers
- Krylov coarse grid solver



Mesh I	Mesh 2	Mesh 3	
256 x 32 x 128	512 x 64 x 256	1024 x 128 x 512	
64 x 16 x 32	128 x 32 x 64	256 x 64 x 128	
32 x 16 x 16	64 x 32 x 32	128 x 64 x 64	
30 million DOFs	237 million DOFs	1.9 billion DOFs	

• Results presented were performed using "Kraken" [Cray XT5]

Rifting at Scale

Mesh I 256 x 32 x 128 30 million DOFs **Mesh 2** 512 x 64 x 256 237 million DOFs Mesh 3 1024 x 128 x 512 1.9 billion DOFs



CPU time (sec) per iteration of Stokes problem, I5-20 iterations required per Newton step

	cores	Linear	Picard
Mesh I	512	3.57	3.88
Mesh 2	4096	8.48	5.90
Mesh 3	32786	7.86	7.12

cores	Linear	Picard		
2048	2.04	2.22		
6384	4.56	4.7 I		
strong scaling				

weak scaling

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Rifting at Scale

Mesh I 256 x 32 x 128 30 million DOFs **Mesh 2** 512 x 64 x 256 237 million DOFs Mesh 3 1024 x 128 x 512 1.9 billion DOFs



CPU time (sec) per *iteration* of Stokes problem, 15-20 iterations required per Newton step

	cores	Linear	Picard	cores	Linear	Picard
Mesh I	512	3.57	3.88	2048	2.04	2.22
Mesh 2	4096	8.48	5.90	16384	4.56	4.71
Mesh 3	32786	7.86	7.12	strong scaling		
weak scaling						

- Fixed three level hierarchy obviously prohibits possibility of perfect weak scaling, however 8 times larger problems requires < 2 times more CPU time.
- Strong scaling is in the range of 20-43% efficiency. Strongly influenced by massively parallel, small sub-domain coarse grid solver.
- Performing non-linear, high resolution 3D thermo-mechanically coupled visco-plastic (non-trivial) simulations is still challenging.

Conclusions and Outlook

- I. Matrix Free (MF) SpMV kernels for Q2 elements reduce memory foot print, avoid the memory bandwidth bottleneck and thus scale well on parallel multi-core architectures
- 2. MF operators combined with Chebyshev/Jacobi can result in robust and efficient parallel MG smoothers for VV Stokes
- 3. Hybrid coarsening strategies can yield significant speed gains for "hard" problems
- 4. The distributed coarse grid solver is a scalability bottleneck. Further experimentation using (i) semi-redundant solves, (ii) AMG coarse grid solvers and (iii) Krylov methods with non-blocking global reductions needs to be conducted
- 5. Usage of hybrid MPI-OpenMP parallelism needs to be investigated

Thanks for your attention...questions?



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