Mathematica® and COMSOL Multiphysics®: A Powerful Workflow for Creating General FE Formulations

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Acknowledgments

Collaborators

- Ravi T. Kedarasetti, Ph.D. Candidate, Center for Neural Engineering, Penn State
- Nitesh Nama, former Ph.D. student now a postdoc at the University of Michigan.
- Eric Abercrombie, recently graduated M.S. student

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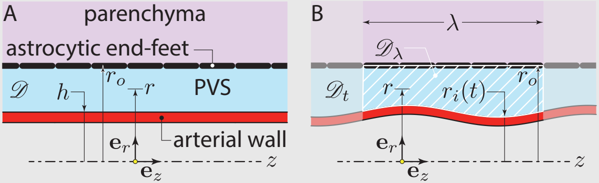
Motivation

- Our workplace: **Penn State Center for Neural Engineering**
- Current projects:
  - Microacoustofluidic mixers/cell manipulation
  - Metabolite exchange in brain
  - Acute stroke: blood clotting/lysis, embolization, clot removal
  - Biodegradation of tissue engineered scaffolds
- Math/computation interests:
  - Mixture theory
  - Traditional and complex fluid flow with fluid-structure interaction and stabilization
  - large-strain poroelasticity
  - Reaction-diffusion-advection
- **Need**: to **quickly** develop accurate and reliable multiphysics numerical schemes
- **Preferred tool**: the **Mathematics Interfaces** in COMSOL Multiphysics — we can focus on FE formulations and stabilization and spend less time in low-level programming
- **Main obstacle**: typying very complex formulations into COMSOL without typographical errors.
- **Solution**: **We leaned on Wolfram's Mathematica** — combining Mathematica and COMSOL opened the door to significant progress for us and this presentation is meant to tell you about our experience.

VMM-Stabilized ALE Formulation of Darcy-Brinkman Flow in Axisymmetric Geometry

An example



Strong form: $\underbrace{\frac{\epsilon\mu}{\kappa}(\mathbf{v}-\mathbf{v}_m)+\nabla p-\nabla\cdot[2\mu(\nabla\mathbf{v})_{\mathrm{sym}}]-\mathbf{b}}_{\mathbf{r}\text{: residual}}=\mathbf{0}$ and $\nabla\cdot\mathbf{v}-q=0$ in $\mathscr{D}_\lambda$

Stabilized weak form with companion fine-scale problem:

$$\left(\tilde{\mathbf{v}},\frac{\epsilon\mu}{\kappa}(\mathbf{v}-\mathbf{v}_m)-\mathbf{b}\right)+(\nabla\tilde{\mathbf{v}},\boldsymbol{\sigma})+(\tilde{p},\nabla\cdot\mathbf{v}-q)+(\boldsymbol{\phi},\boldsymbol{\tau}\mathbf{r})=0,\quad \boldsymbol{\sigma}=-p\mathbf{I}+2\mu(\nabla\mathbf{v})_{\mathrm{sym}},$$

$$\boldsymbol{\phi}=-\frac{\epsilon\mu}{\kappa}\tilde{\mathbf{v}}+\nabla\cdot[\tilde{p}\mathbf{I}+2\mu(\nabla\tilde{\mathbf{v}})_{\mathrm{sym}}],\quad \left(\tilde{\boldsymbol{\tau}}\mathbf{w}_i,\frac{\epsilon\mu}{\kappa}\mathbf{w}_i-\mathbf{w}_i\right)+([\nabla(\tilde{\boldsymbol{\tau}}\mathbf{w}_i)]_{\mathrm{sym}},2\mu[\nabla(\boldsymbol{\tau}\mathbf{w}_i)]_{\mathrm{sym}})=0,$$

with $\mathbf{w}_1=-\mathbf{e}_r$ and $\mathbf{w}_2=-\mathbf{e}_z$. **Boundary conditions:** $\mathbf{v}$ given at the inner and outer radii; λ-periodicity; zero-pressure average. The $\boldsymbol{\tau}$ problem is posed in a space of bubble functions.

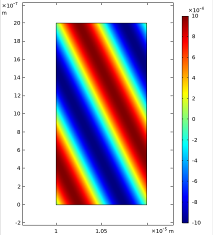
These equations hold over the (deformed) physical domain: They must be pulled back to the computational domain — remapping second order differential operators: chain rule galore.

VMM-Stabilized ALE Formulation of Darcy-Brinkman Flow in Axisymmetric Geometry

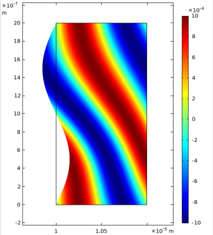
Convergence Study with the Method of Manufactured Solutions

- Figures: **Method of Manufactured Solutions**, radial velocity component.
- Application interest: flow of interstitial fluid in the paravascular space of the brain.
- ALE: Arbitrary Lagrangian–Eulerian
  - Physical domain $\neq$ computational domain
  - **Eqs. are complex on the solution's domain**
  - **Eqs. are "simple" on the physical domain**
- VMM: **Virtual Multiscale Method**

  [for Darcy-Brinkman flow, see A. Masud, IJNMF, **54**(2007), pp. 665–681]
- **VMM "Cost"**
  - Needs the residual (2nd order derivatives).
  - Needs an auxiliary (stabilization) field $\boldsymbol{\tau}$.
- **VMM "Benefits"**
  - Strongly consistent
  - Effective in convection-dominated problems
  - Computing $\boldsymbol{\tau}$ is **transparent** (cf. SUP/G)
  - **Lessens the restrictions of the inf-sup condition**



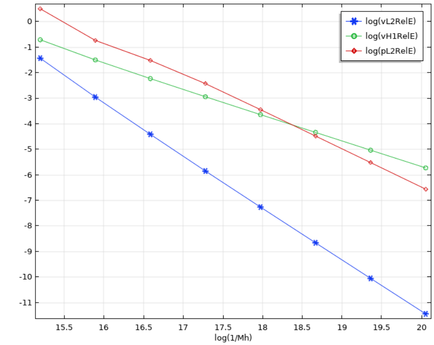
v_r in the computational domain



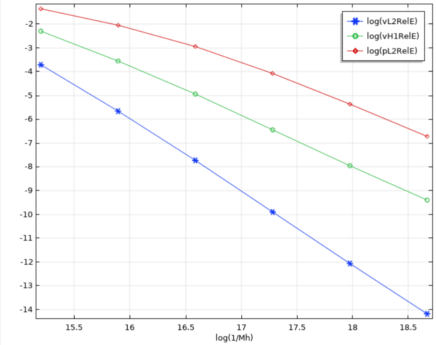
v_r in the physical domain

Example: Convergence Study

- **FE Grid**: squares with side of length **Mh**.
- Parametric sweep over a range of values for Mh.



Q1 elements for p and $\mathbf{v}$.
Cubic bubbles for $\boldsymbol{\tau}$. 8 cycles of uniform refinement. Maximum number of dofs.: 1,577,475. Duration: 105 s on my MacBook Pro.

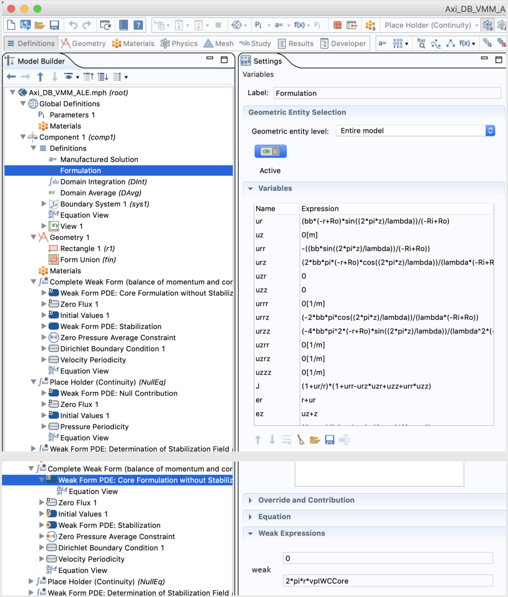


Q2 elements for p and $\mathbf{v}$.
Cubic bubbles for $\boldsymbol{\tau}$. 6 cycles of uniform refinement. Maximum number of dofs.: 395,523. Duration: 25 s, again on my MacBook Pro.

How Were the Calculations Done?

COMSOL's powerful input syntax

- COMSOL provides **Mathematics Interfaces**
- Interfaces we typically use:
  - Weak Form PDE
  - ODE and DAE
- Our "standard approach":
  - **Component Node**: add a physics using a Mathematics Interface — (typically) this instantiates a FE field
  - **Definitions sub-node**: add **Variables Table(s)**: **it is here that we define the formulation expressions**
  - We invoke one such definitions in the appropriate equation interface.
- **We do NOT type definitions**: **we import them from text file(s)**
- **We create the text files using Mathematica**



Quick Reminder about COMSOL's Syntax

- Default coordinate system in COMSOL:
  - Cartesian: (x, y, z)
  - Cylindrical: (r, phi, z)
- **COMSOL allows a user to label an FE field as a whole and to independently name the field's components**. For example, let "$vector\_u$" be the label for a vector-valued field in 3D. We can then name the components $(first, second, third)$.
  - If, say, we are using (x, y, z) for the coordinates, it may make more sense to name the vector components (ux, uy, uz) — again, these are just names.
- Once names are given, COMSOL has an intuitive syntax to refer to derivatives:

$$\frac{\partial uy}{\partial x} \to uyx, \quad \frac{\partial^3 ux}{\partial y \partial z^2} \to uxyzz, \quad \frac{\partial uz}{\partial t} \to uzt, \quad \text{etc.}$$

- Note: time derivatives must go last.
- The test functions associated to a particular field are invoked by simply setting the field in question as the argument of the `test( )` operator.
- So, what does the input for our VMM-stablized Example look like? . . . Let's consider a very simple example first . . .

Input for 3D Elastodynamics

```
IWC
(-bx+rho*uxtt)*test(ux)+(2*mu*uxx+lambda*(uxx+uyy+uzz))*test(uxx)+(-by+
rho*uytt)*test(uy)+mu*(uxy+uyx)*(test(uxy)+test(uyx))+(2*mu*uyy+lambda*(
uxx+uyy+uzz))*test(uyy)+(-bz+rho*uztt)*test(uz)+mu*(uxz+uzx)*(test(uxz)+
test(uzx))+mu*(uyz+uzy)*(test(uyz)+test(uzy))+(2*mu*uzz+lambda*(uxx+uyy+
uzz))*test(uzz)
BWC -(sx*test(ux))-sy*test(uy)-sz*test(uz)
Energy
(lambda*(uxx+uyy+uzz)^2+mu*(2*uxx^2+(uxy+uyx)^2+2*uyy^2+(uxz+uzx)^2+(uyz
+uzy)^2+2*uzz^2))/2.
exx uxx
exy (uxy+uyx)/2.
exz (uxz+uzx)/2.
eyx (uxy+uyx)/2.
eyy uyy
eyz (uyz+uzy)/2.
ezx (uxz+uzx)/2.
ezy (uyz+uzy)/2.
ezz uzz
sxx (exx+eyy+ezz)*lambda+2*exx*mu
sxy 2*exy*mu
sxz 2*exz*mu
syx 2*eyx*mu
syy (exx+eyy+ezz)*lambda+2*eyy*mu
syz 2*eyz*mu
szx 2*ezx*mu
szy 2*ezy*mu
szz (exx+eyy+ezz)*lambda+2*ezz*mu
```

- Define a single physics with a vector-valued displacement field $\mathbf{u}$.
- Components of $\mathbf{u}$: (ux, uy, uz).
- The weak form of the linear elastic BVP is

$$(\tilde{\mathbf{u}}, \partial_{tt}\mathbf{u} - \mathbf{b}) + ([\nabla\tilde{\mathbf{u}}]_{\mathrm{sym}}, \boldsymbol{\sigma}) - (\tilde{\mathbf{u}}, \mathbf{s})_{\Gamma_N} = 0$$

$$\boldsymbol{\sigma} = 2\mu\boldsymbol{\varepsilon} + \lambda(\operatorname{tr}\boldsymbol{\varepsilon})\mathbf{I}$$

$$\boldsymbol{\varepsilon} = (\nabla\mathbf{u})_{\mathrm{sym}}$$

  λ and μ are the Lamè elastic constants (moduli).
- Boundary conditions: $\mathbf{u} = \mathbf{u}_0$ on Γ_D and $\boldsymbol{\sigma}\mathbf{n} = \mathbf{s}$ on Γ_N, with Γ_D and Γ_N the Dirichlet and the Neumann parts of the boundary.

Input for the VMM-Stabilized Porous Flow Example

Actually, only one term . . .

Definition of the stabilization term:

```
StabilizationIWC
J*((taurr*(-br+pr*rer+(2*muB*vr)/er^2+(epsilon*muD*vr)/kappa+pz*zer-(2*
muB*(rer*vrr+vrz*zer))/er-muB*(2*rerer*vrr+rezez*vrr+2*rer^2*vrrr+rez^2*
vrrr+rerez*vzr+rer*rez*vzrr+4*rer*vrrz*zer+rez*vzrz*zer+2*vrzz*zer^2+2*
vrz*zerer+vzz*zerez+2*rez*vrrz*zez+rer*vzrz*zez+vzzz*zer*zez+vrzz*zez^2+
vrz*zezez))+taurz*(-bz+pr*rez+(epsilon*muD*(c+vz))/kappa+pz*zez-(muB*(
rez*vrr+rer*vzr+vzz*zer+vrz*zez))/er-muB*(rerez*vrr+rerer*vzr+rer^2*vzrr
+rez*vrrz*zer+vzzz*zer^2+vzz*zerer+vrz*zerez+vrzz*zer*zez+rer*(rez*vrrr+
2*vzrz*zer+vrrz*zez))-2*muB*(rezez*vzr+rez^2*vzrr+2*rez*vzrz*zez+vzzz*
zez^2+vzz*zezez)))*(rer*test(pr)+zer*test(pz)-(epsilon*muD*test(vr))/
kappa+(2*muB*(-test(vr)+er*rer*test(vrr)+er*zer*test(vrz)))/er^2+2*muB*(
rerer*test(vrr)+rer^2*test(vrrr)+2*rer*zer*test(vrrz)+zerer*test(vrz)+
zer^2*test(vrzz))+muB*(rezez*test(vrr)+rez^2*test(vrrr)+2*rez*zez*test(
vrrz)+zezez*test(vrz)+zez^2*test(vrzz)+rerez*test(vzr)+rer*rez*test(vzrr
)+rez*zer*test(vzrz)+rer*zez*test(vzrz)+zerez*test(vzz)+zer*zez*test(
vzzz)))+(tauzr*(-br+pr*rer+(2*muB*vr)/er^2+(epsilon*muD*vr)/kappa+pz*zer
-(2*muB*(rer*vrr+vrz*zer))/er-muB*(2*rerer*vrr+rezez*vrr+2*rer^2*vrrr+
rez^2*vrrr+rerez*vzr+rer*rez*vzrr+4*rer*vrrz*zer+rez*vzrz*zer+2*vrzz*zer
^2+2*vrz*zerer+vzz*zerez+2*rez*vrrz*zez+rer*vzrz*zez+vzzz*zer*zez+vrzz*
zez^2+vrz*zezez))+tauzz*(-bz+pr*rez+(epsilon*muD*(c+vz))/kappa+pz*zez-(
muB*(rez*vrr+rer*vzr+vzz*zer+vrz*zez))/er-muB*(rerez*vrr+rerer*vzr+rer^2
*vzrr+rez*vrrz*zer+vzzz*zer^2+vzz*zerer+vrz*zerez+vrzz*zer*zez+rer*(rez*
vrrr+2*vzrz*zer+vrrz*zez))-2*muB*(rezez*vzr+rez^2*vzrr+2*rez*vzrz*zez+
vzzz*zez^2+vzz*zezez)))*(rez*test(pr)+zez*test(pz)-(epsilon*muD*test(vz)
)/kappa+(muB*(rez*test(vrr)+zez*test(vrz)+rer*test(vzr)+zer*test(vzz)))/
er+muB*(rerez*test(vrr)+rer*rez*test(vrrr)+rez*zer*test(vrrz)+rer*zez*
test(vrrz)+zerez*test(vrz)+zer*zez*test(vrzz)+rerer*test(vzr)+rer^2*test
(vzrr)+2*rer*zer*test(vzrz)+zerer*test(vzz)+zer^2*test(vzzz))+2*muB*(
rezez*test(vzr)+rez^2*test(vzrr)+2*rez*zez*test(vzrz)+zezez*test(vzz)+
zez^2*test(vzzz))))
```

I did not type this, Mathematica did!

- The whole formulation is contained in a single text file with 4776 characters, forming 1045 “words”, over 30 lines — the line to the left has 2007 characters
- This is not the most complex input we asked COMSOL to read
- The COMSOL parser is very resilient
- The true limitation is on the part of the user when he/she might need to debug errors

Let’s see how this is created with Mathematica . . .

Reduced Coordinates

Weak Forms

$$\left(\tilde{\mathbf{v}}, \frac{\epsilon\mu}{\kappa}(\mathbf{v}-\mathbf{v}_m)-\mathbf{b}\right)+(\nabla\tilde{\mathbf{v}},\boldsymbol{\sigma})+(\tilde{p},\nabla\cdot\mathbf{v}-q)+(\boldsymbol{\phi},\boldsymbol{\tau}\mathbf{r})=0, \quad \boldsymbol{\sigma}=-p\mathsf{I}+2\mu(\nabla\mathbf{v})_{\mathrm{sym}},$$

$$\boldsymbol{\phi}=-\frac{\epsilon\mu}{\kappa}\tilde{\mathbf{v}}+\nabla\cdot[\tilde{p}\mathsf{I}+2\mu(\nabla\tilde{\mathbf{v}})_{\mathrm{sym}}], \quad \left(\tilde{\boldsymbol{\tau}}\mathbf{w}_i, \frac{\epsilon\mu}{\kappa}\mathbf{w}_i-\mathbf{w}_i\right)+([\nabla(\tilde{\boldsymbol{\tau}}\mathbf{w}_i)]_{\mathrm{sym}}, 2\mu[\nabla(\boldsymbol{\tau}\mathbf{w}_i)]_{\mathrm{sym}})=0,$$

Balance of Momentum and Continuity Equation: Core without VMM stabilization

Expression of the residual

```
In[34]:= Residual = (epsilon muD / kappa) (vF - vm) - bF - Div[σ[pF, vF], ECoordinates, "Cylindrical"];
```

Stabilization test function

```
In[35]:= AdjointTestStress = test[pF] × IdentityMatrix[3] +
           2 muB Sym[Grad[test[vF], ECoordinates, "Cylindrical"]];

In[36]:= StabilizationTestFunction =
          - (epsilon muD / kappa) test[vF] + Div[AdjointTestStress, ECoordinates, "Cylindrical"];
```

Stabilization contribution to weak form

```
In[37]:= StabilizationIWCLong = J IP[StabilizationTestFunction, tauF.Residual];

In[38]:= StabilizationIWC =
          Simplify[Compactify[Compactify[StabilizationIWCLong, RLECoordinates], RECoordinates]]
```

no other

Mathematica COMSOL Support Package

Key features

- Our Mathematica package allows one to mimic the "paper and pencil" equations
- We stuck to using Mathematica's native differential operators:
  - **ALE formulations are automatically built via the chain rule!**
  - No limit to the order of differentiation: **determination of residuals for in any coordinate system**
- To use Mathematica's native differential operators, the relevant fields must be written as functions of the coordinates: **This is not allowed in COMSOL**. **Therefore, we created a function called `Compactify[]` to convert Mathematica expressions into COMSOL-compatible equivalents.**
- When solving for the gradients of an inverse ALE Map we rely on the Mathematica's native `Solve[]` function.
- We created a `test[]` operator to imitate the required syntax in COMSOL.
- We created a function called `COMSOLForm[]` as an extension of Mathematica's native `FortranForm[]` to translate Mathematica's expressions into compatible COMSOL definitions.

Package Function List

Here is the full list of the functions in our COMSOLSupport Package

- `IP[*,*]`: generalized inner product
- `Sym[*]`: symmetrization of 2nd order tensors
- `COMSOLProblemSettings[---]`: Initialization of problem type, dimension, coordinate system, naming convention
- `test[*]`: a linear operator obeying the product rule, commuting with differential operators
- `DInt[*]`: a mere wrapper standing for "domain integration"; **must be defined in COMSOL**
- `Tensorify[*,*,*]`: creates an expression representing a tensor of specified order
- `Functionify[*,*]`: turns a symbol into a function of specified arguments
- `Fieldfy[*,*]`: an alias for `Functionify[*,*]`
- `Testify[*]`: alternative to `test[*]` treating test functions as functions
- `Compactify[*,*]`: transform expression functions of specified coordinates into COMSOL-compatible expressions.
- `ClearOutputFiles[*]`: simple file initialization
- `COMSOLExport[*,*]`: writes COMSOL-compatible expressions to a textfile
- `COMSOLForm[*]`: turns a Mathematica expression into one interpretable by the COMSOL parser
- `COMSOLRule[*,*]`: defines the pairs to appear in a COMSOL definition table.

Summary

- Research support mission: rapid deployment of schemes not normally available in ready-made computational packages
- COMSOL Multiphysics is an ideal tool in creating new FE formulations
- Main stumbling block: the expressions in multiphysics simulations are often very hard to hand-type correctly
- We were able to overcome our difficulties by manipulating complex formulations using Mathematica
- We formalized our workflow into a Mathematica Package that has proven to be very versatile and (relatively) easy to use even in the most complex formulations we have worked on so far.
- We will make our Mathematica package and accompanying examples available as a Git repository hosted on GitHub
- Please contact me (Francesco Costanzo) at **fxc8@psu.edu** is you are interested

Any questions?