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School of Computing
Scientific Computation Group

Towards the development and application of an optimal solver for continuum models of tumour growth

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Motivations

Ultimate goal is to solve complex non-linear parabolic systems by applying:

- adaptive meshing,
- second order Backward Differentiation Formula (BDF) 2 temporal scheme,
- non-linear multigrid method,
- parallel technique.

Outline

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- Non-linear multigrid
- Cahn-Hilliard-Hele-Shaw (CHHS) system of equations
- Improved solver for CHHS system of equations
- Model of thin film flows
- Adaptive meshing on droplet
- Tumour model from S.M. Wise et al.
- Future plan

Non-linear multigrid

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- Full Approximate Storage (FAS) scheme
- for problem on fine grid:
  - $A(\underline{u}^f) = \underline{b}^f$
  - $r^f = \underline{b}^f - A(\underline{u}^*)$
- for coarse grid correction:
  - $A(\underline{u}^c) = \underline{b}^c + [I_f^c \underline{r}^f - (\underline{b}^c - A(I_f^c \underline{u}^*))]$
  - $\underline{e}^{\text{correction}} = \underline{u}^c - \underline{u}^*$

CHHS system of equations

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$$
\begin{aligned}
\partial_t \phi &= \Delta \mu - \nabla \cdot (\phi \mathbf{u}) \\
\mathbf{u} &= -\nabla p - \gamma \phi \nabla \mu \\
\nabla \cdot \mathbf{u} &= 0 \\
\mu &= \phi^3 - \phi - \epsilon^2 \Delta \phi
\end{aligned}
$$

with Neumann boundary conditions:

$$\partial_n \phi = 0 \quad \partial_n \mu = 0 \quad \partial_n p = 0 \text{ on } \partial\Omega$$

S. M. Wise, J. Sci. Comput, 44: 38-68, 2010.

Our solver

- Cell-centred 2^{nd} order finite difference method on rectangular grids
- PARAMESH library for mesh generation
- Fully implicit 2^{nd} order discretization in time (BDF2)
- FAS multigrid at each time-step
- Newton-block 3×3 Red-Black (weighted) Gauss-Seidel smoother
- Full weighting restriction and multi-linear interpolation

CHHS system of equation

Level of grids	degrees of freedom	max No. V-cycle from our solver	max No. V-cycle from Wise's solver
2	4096	8	8
3	16,384	9	9
4	65,536	10	9
5	262,144	10	10
6	1,048,576	10	11

Optimal multigrid performances from our BDF2 solver and Wise's solver with semi-implicit scheme.

CHHS system of equation

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Level of grids	number of time-steps	L_∞ error in ϕ from our solver	ratio	L_∞ error in ϕ from Wise's solver	ratio
2	80	-	-	-	-
3	160	2.139E-003	-	2.954E-002	-
4	320	5.379E-004	3.977	1.151E-002	2.566
5	640	1.347E-004	3.993	5.011E-003	2.297
6	1280	3.370E-005	3.997	2.333E-003	2.148

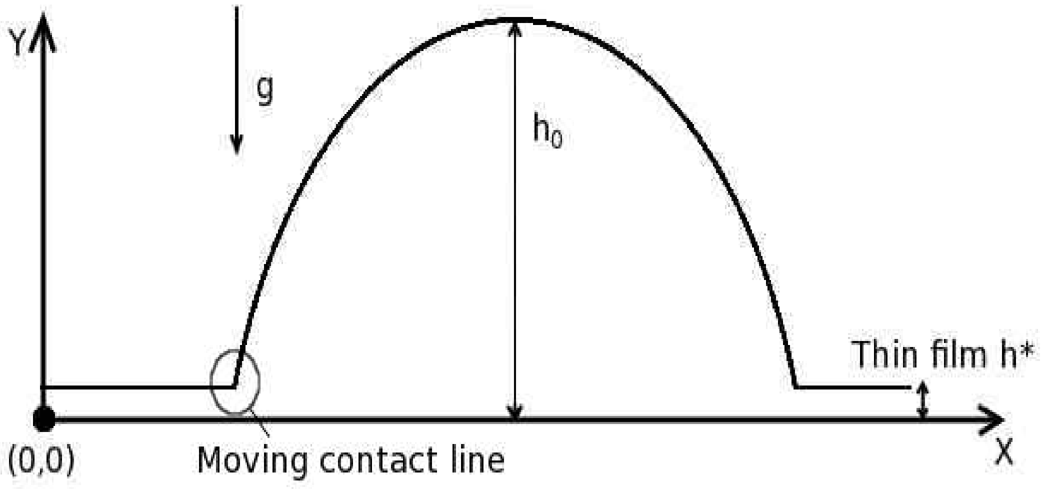
Convergence tests from our BDF2 solver
and Wise's solver with semi-implicit scheme.

Droplet Spreading Flow

$$\begin{aligned} \partial_t h &= \nabla \cdot \left(\frac{h^3}{3}\nabla p\right) \\ p &= -\Delta h - \Pi(h) \end{aligned}$$

with Neumann boundary conditions:

$$\partial_n h = 0 \quad \partial_n p = 0 \quad \text{on} \quad \partial\Omega$$



Our solver

- Cell-centred 2^{nd} order finite difference method
- PARAMESH library for mesh generation and adaptivity
- Fully implicit 2^{nd} order discretization in time (BDF2)
- MLAT variation of FAS multigrid at each time-step
- Newton-block 2×2 Red-Black (weighted) Gauss-Seidel smoother
- Full weighting restriction and multi-linear interpolation

Droplet Spreading Flow

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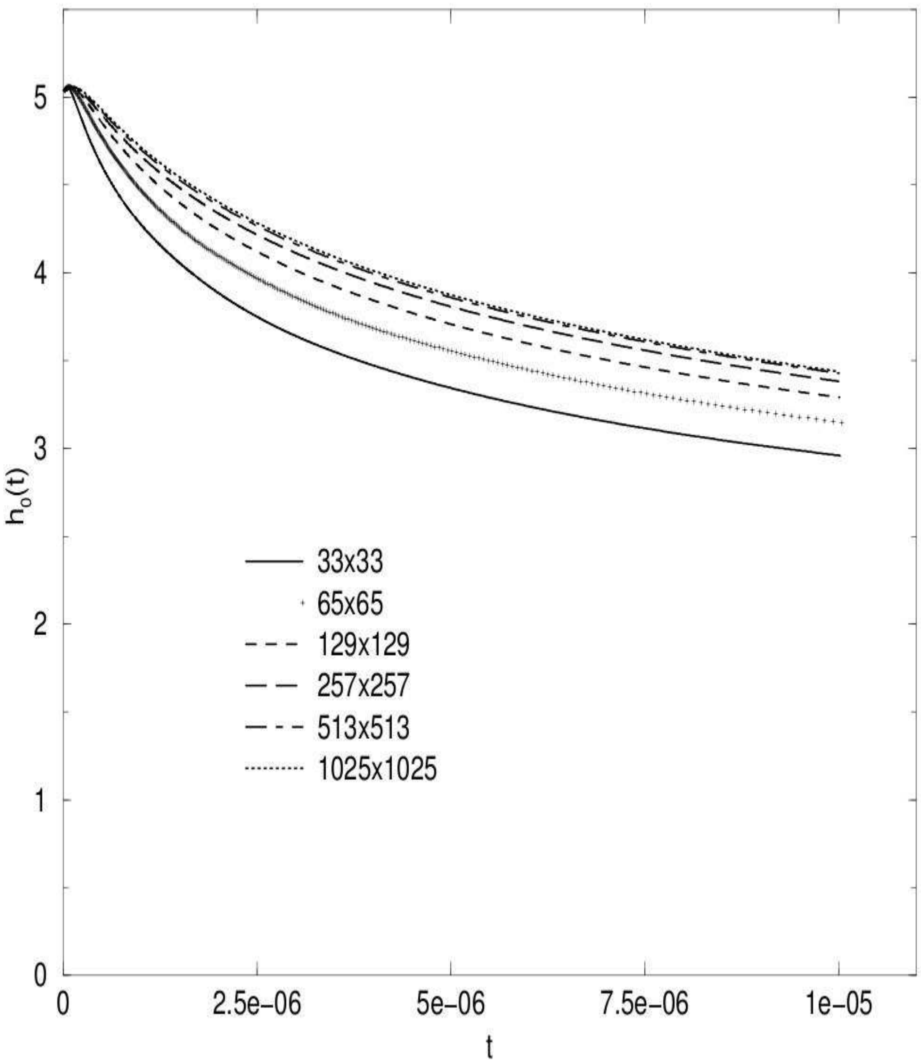
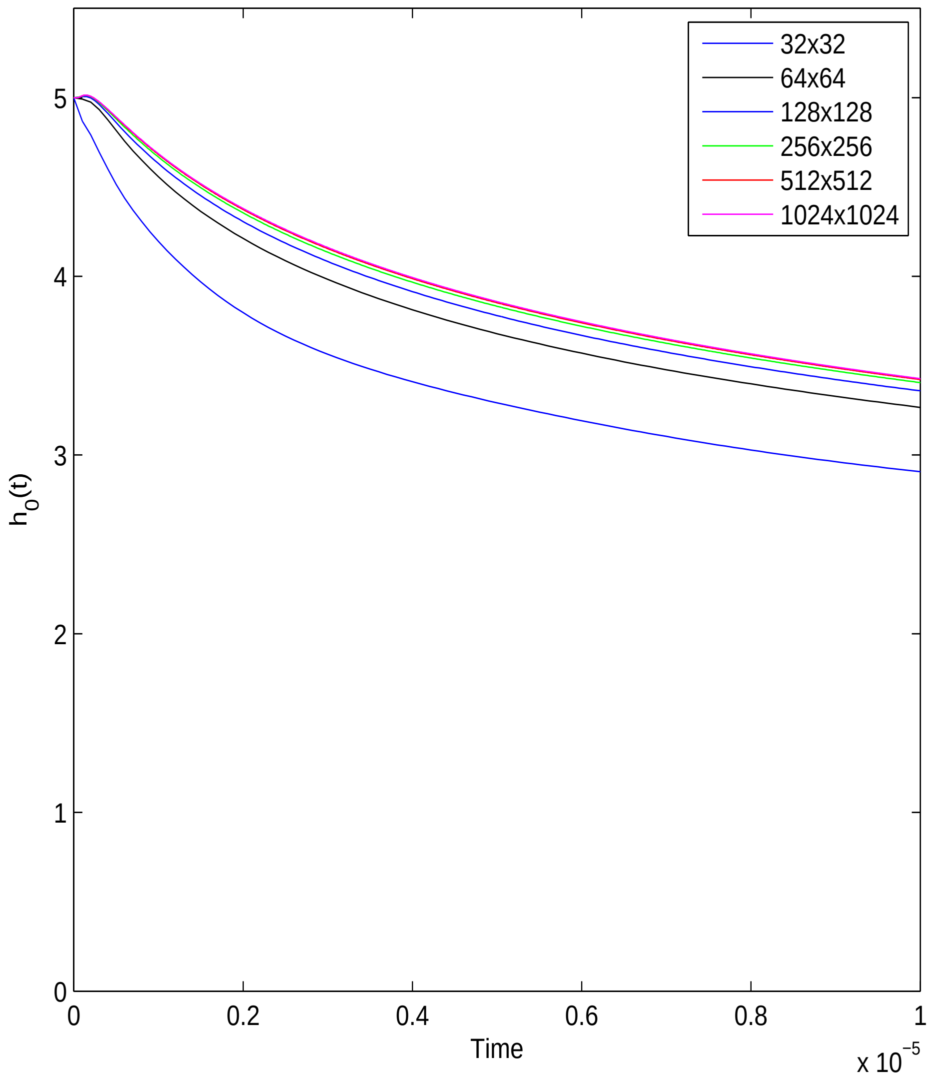


Changes of h from Gaskell et al. (2004)



Changes of h from our solver.

Droplet Spreading Flow

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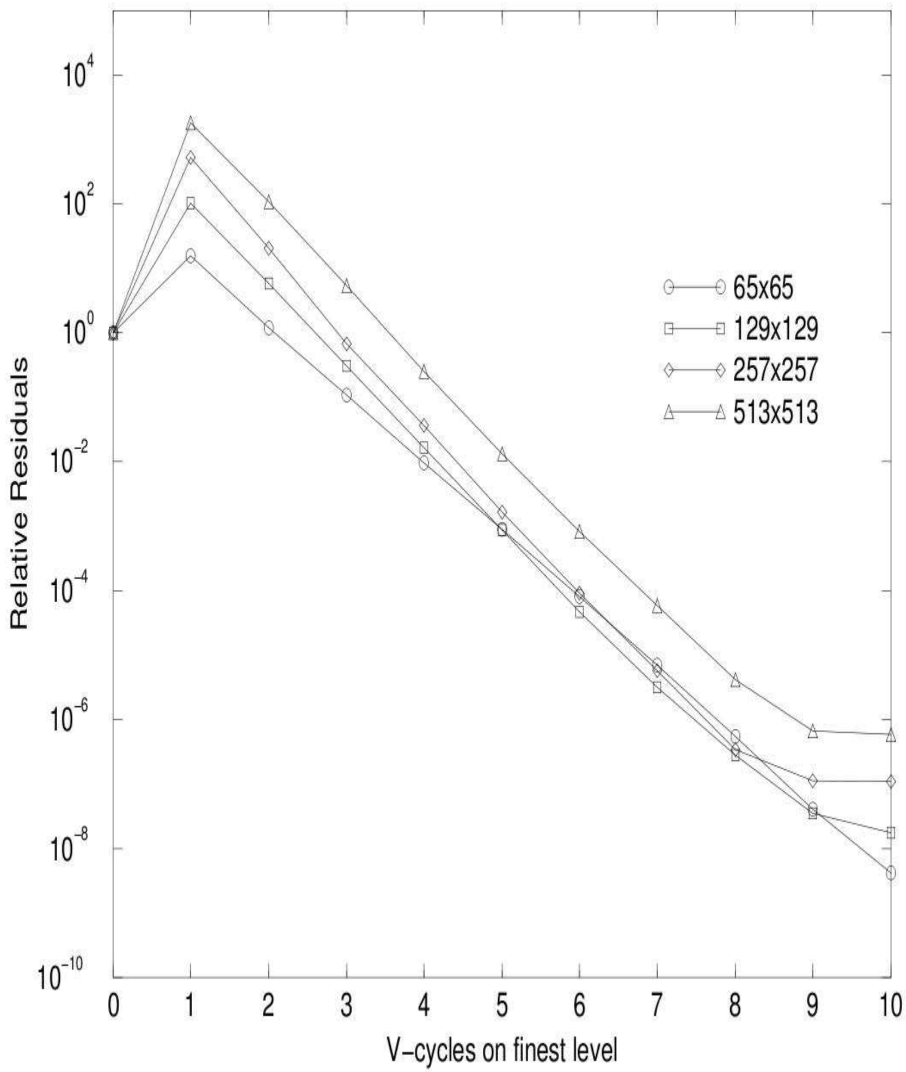
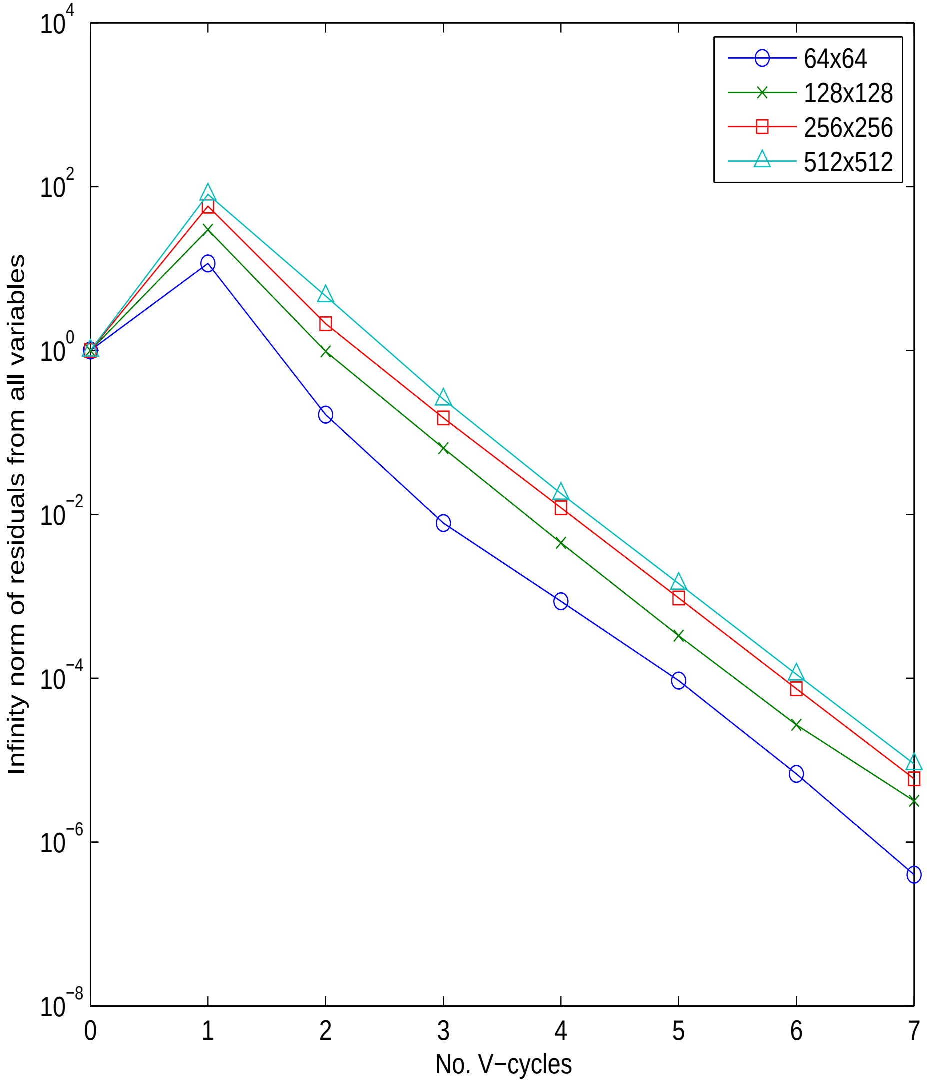
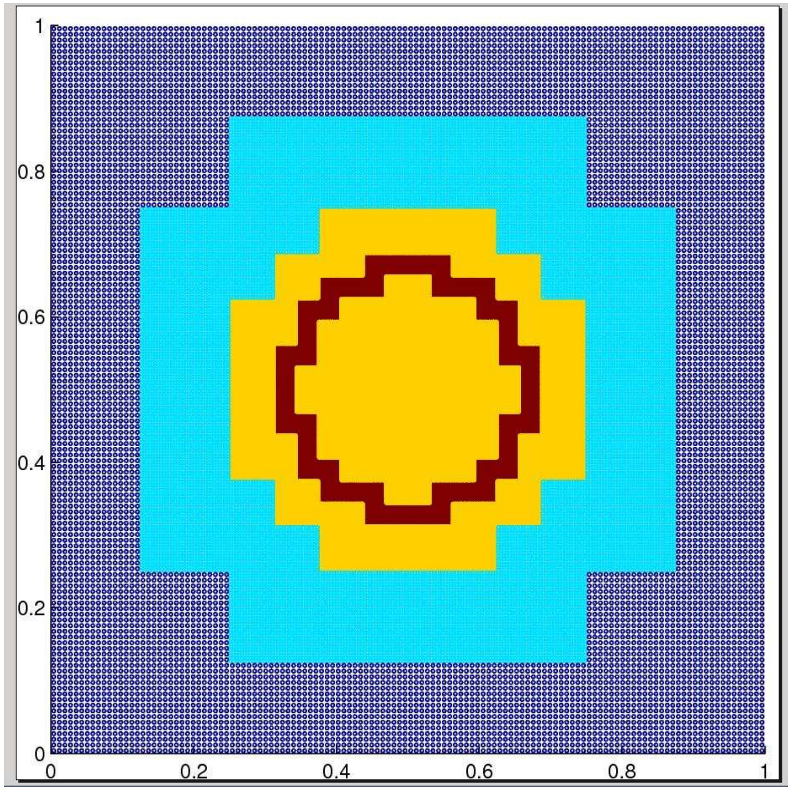


Optimal MG performance from Gaskell et al. (2004)

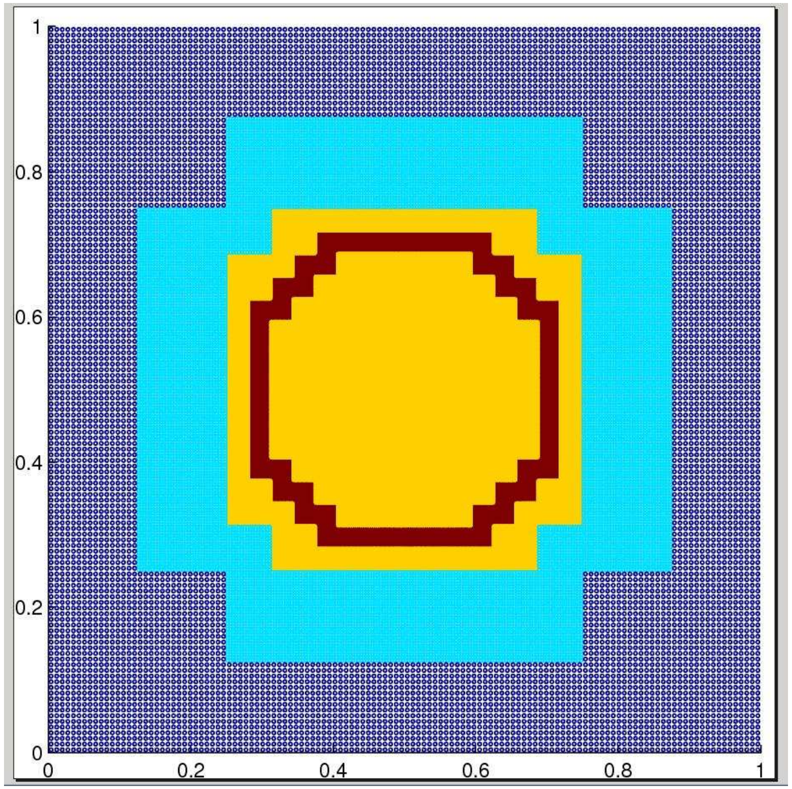


Optimal MG performance from our solver.

Droplet Spreading Flow



Adaptive meshing for initial condition of droplet.



Adaptive meshing at $t = 1 \cdot 10^{-5}$.

Droplet Spreading Flow

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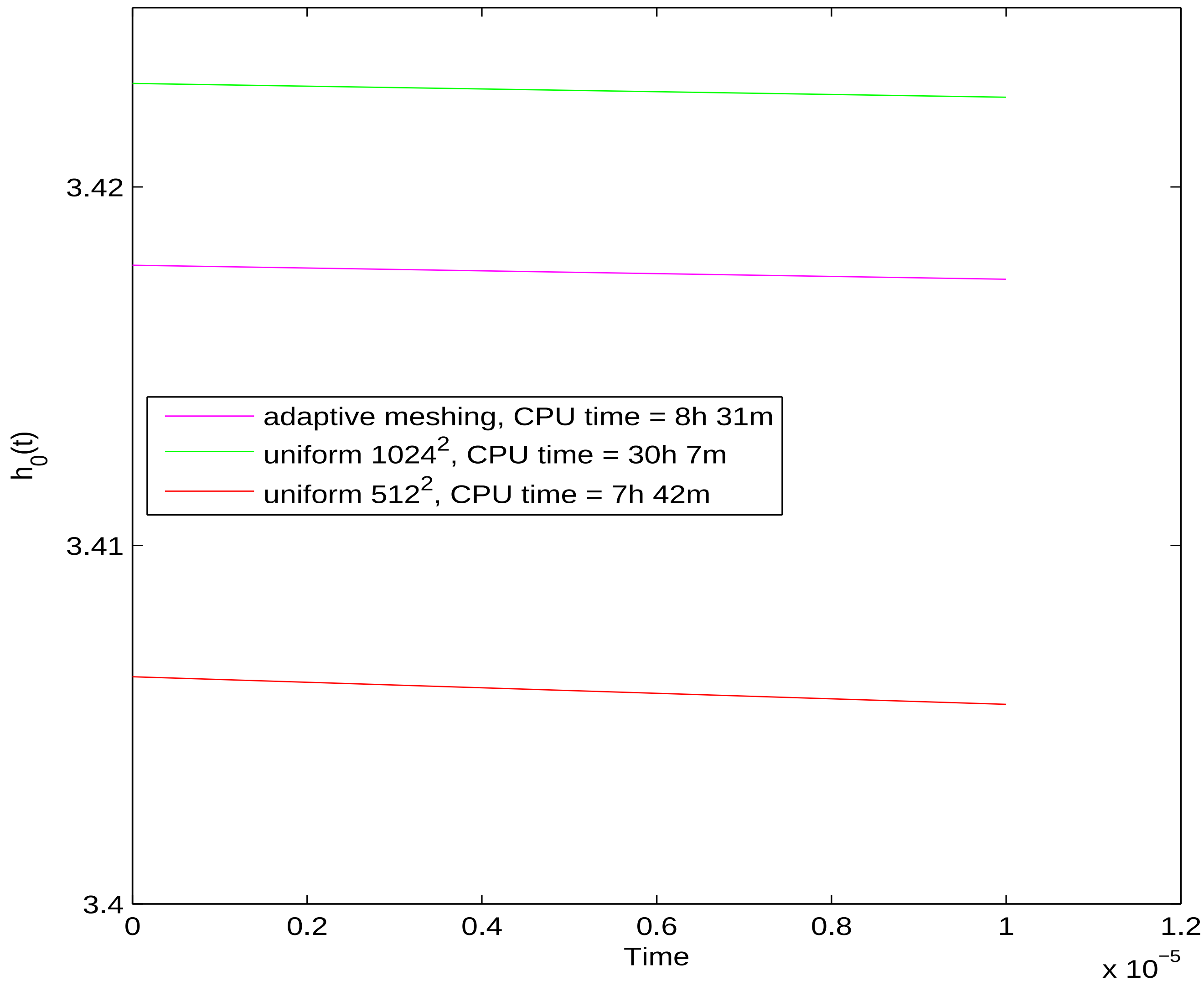

Heights of droplet ($h_0(t)$)

Tumour model from Wise et al.

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$$
\begin{aligned}
\partial_t \phi_T &= M\nabla \cdot (\phi_T \nabla \mu) + S_T(\phi_T, \phi_D, n) - \nabla \cdot (\mathbf{u_S}\phi_T) \\
\mu &= f'(\phi_T) - \epsilon^2 \Delta \phi_T \\
\partial_t \phi_D &= M\nabla \cdot (\phi_D \nabla \mu) + S_D(\phi_T, \phi_D, n) - \nabla \cdot (\mathbf{u_S}\phi_D) \\
\mathbf{u_S} &= -(\nabla p - \frac{\gamma}{\epsilon}\mu \nabla \phi_T) \\
\nabla \cdot \mathbf{u_S} &= S_T(\phi_T, \phi_D, n) \\
0 &= \Delta n + T_C(\phi_T, n) - n(\phi_T - \phi_D)
\end{aligned}
$$

with mixed boundary conditions:

$$\mu = p = 0 \quad n = 1 \quad \underline{\varsigma} \cdot \nabla \phi_T = \underline{\varsigma} \cdot \nabla \phi_D = 0 \quad \text{on} \quad \partial\Omega,$$

S. M. Wise, J. S. Lowengrub, V. Cristini,

Math. Comput. Modelling, 53: 1-20, 2011.

Tumour model from Wise et al.

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$$
\begin{aligned}
\partial_t \phi_T &= M\nabla \cdot (\phi_T \nabla \mu) + S_T(\phi_T, \phi_D, n) - \nabla \cdot (\mathbf{u_S} \phi_T) \\
\mu &= f'(\phi_T) - \epsilon^2 \Delta \phi_T \\
\partial_t \phi_D &= M\nabla \cdot (\phi_D \nabla \mu) + S_D(\phi_T, \phi_D, n) - \nabla \cdot (\mathbf{u_S} \phi_D) \\
[\mathbf{u_S} &= -(\nabla p - \frac{\gamma}{\epsilon} \mu \nabla \phi_T)] \\
-\Delta p &= S_T(\phi_T, \phi_D, n) - \nabla \cdot (\frac{\gamma}{\epsilon} \mu \nabla \phi_T) \\
0 &= \Delta n + T_C(\phi_T, n) - n(\phi_T - \phi_D)
\end{aligned}
$$

with mixed boundary conditions:

$$\mu = p = 0 \quad n = 1 \quad \underline{\varsigma} \cdot \nabla \phi_T = \underline{\varsigma} \cdot \nabla \phi_D = 0 \quad \text{on} \quad \partial\Omega,$$

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Tumour model from Wise et al.

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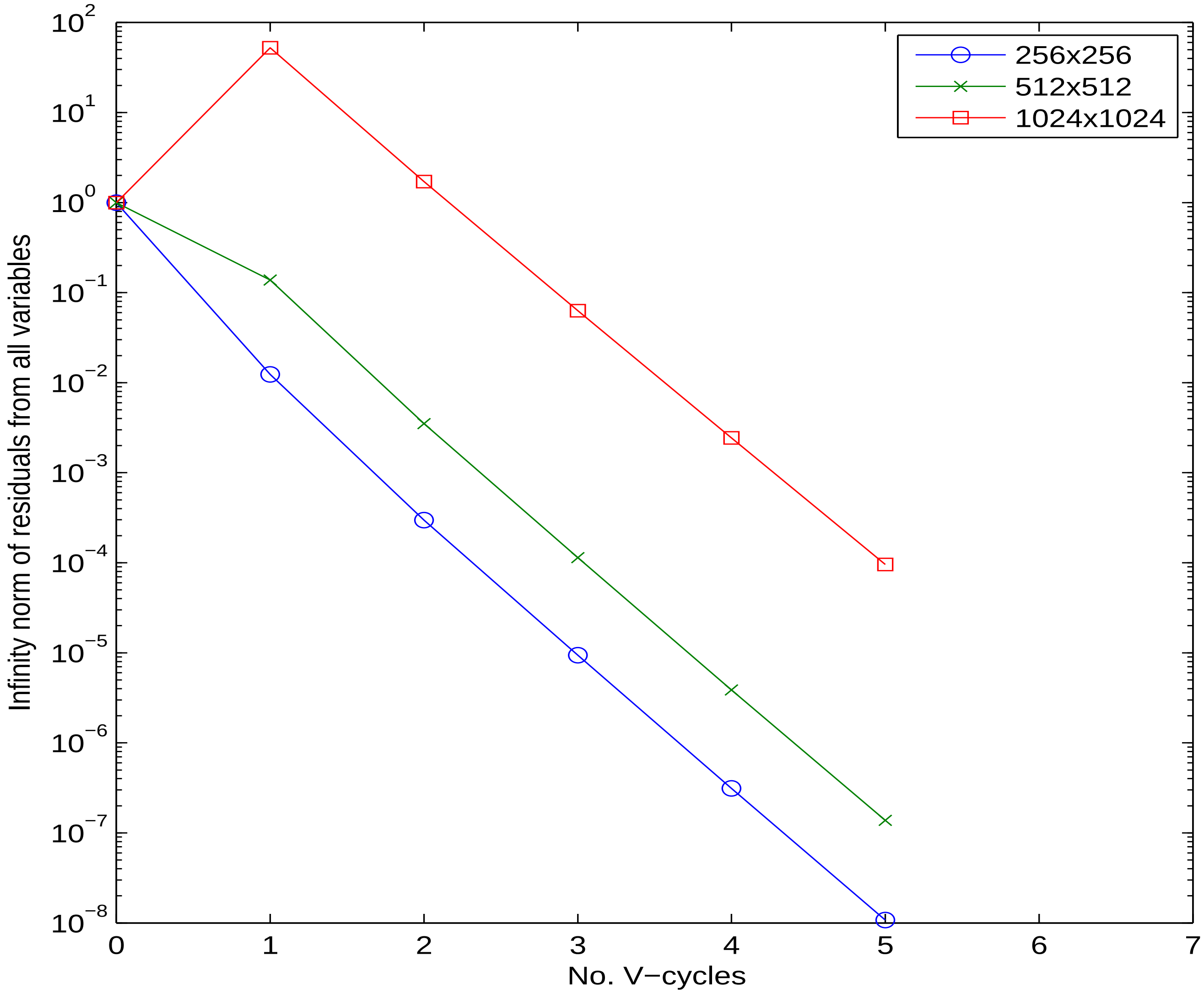

Optimal multigrid convergence on tumour model.

Future plan

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- Validating with results from Wise et al.
- Second order convergence on tumour model
- Adaptive meshing
- Parallel implementation
- 3D