“Development and Application of Parallel Numerical Tools for the Adaptive Multilevel Simulation of Phase-Change Problems”

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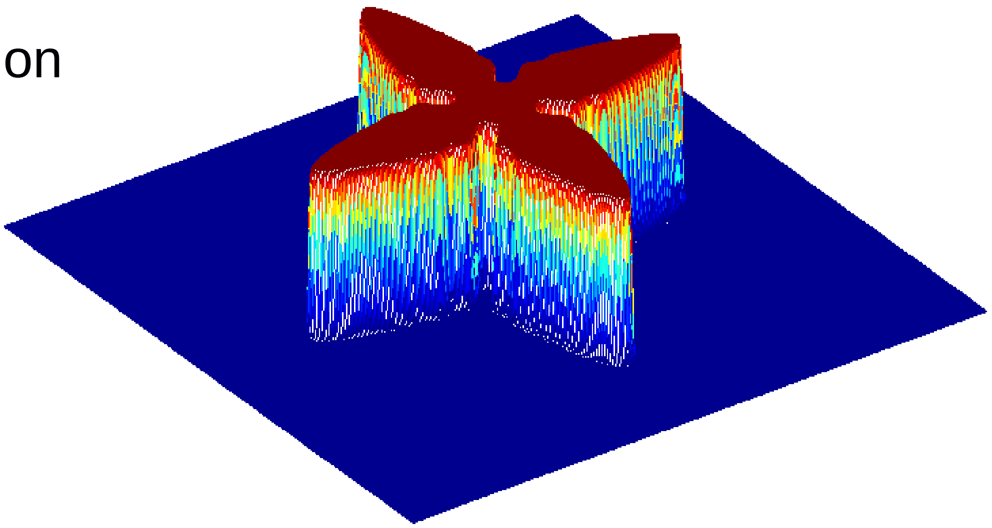
AHPSC, January 2012

Outline

1. Introduction
2. Phase-field models for simulating solidification processes
3. Adaptive spatial discretisation
4. Implicit temporal discretisation
5. Nonlinear multigrid solvers
6. Results in 2-d
7. 3-d parallel implementation
8. Parallel results in 3-d
9. Summary and Discussion

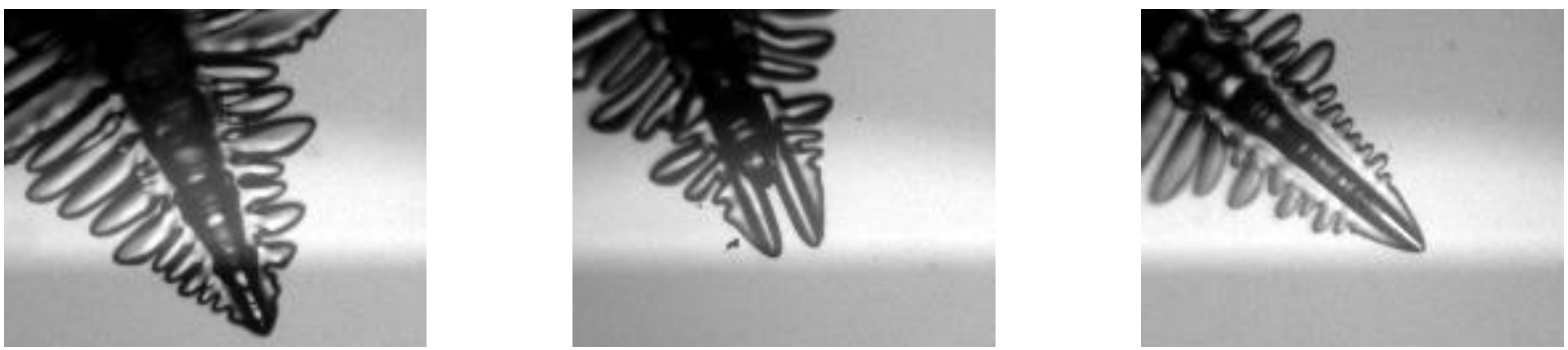


Introduction

• Real Solidification Structures

•One of the most fundamental and important microstructures produced during solidification is the dendrite

•In this work we seek to study these phenomena computationally using both two and three-dimensional models



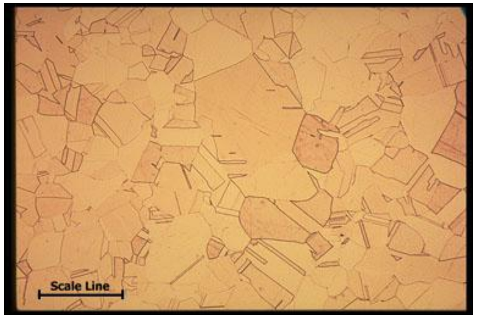
Experimental capture of dendritic microstructure formation in Xenon systems (see, for example, Phys. Rev. E., 54:5309-5326, 1996)

Introduction

• Thermodynamic Background

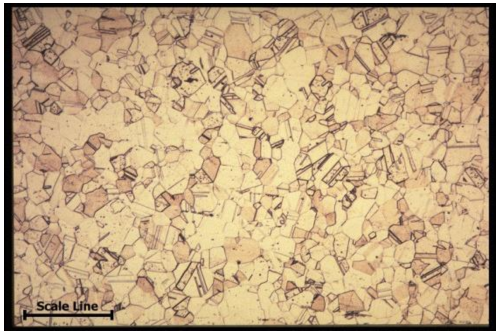
Driving force for Solidification

Pure Materials



Temperature

Alloys



Concentration

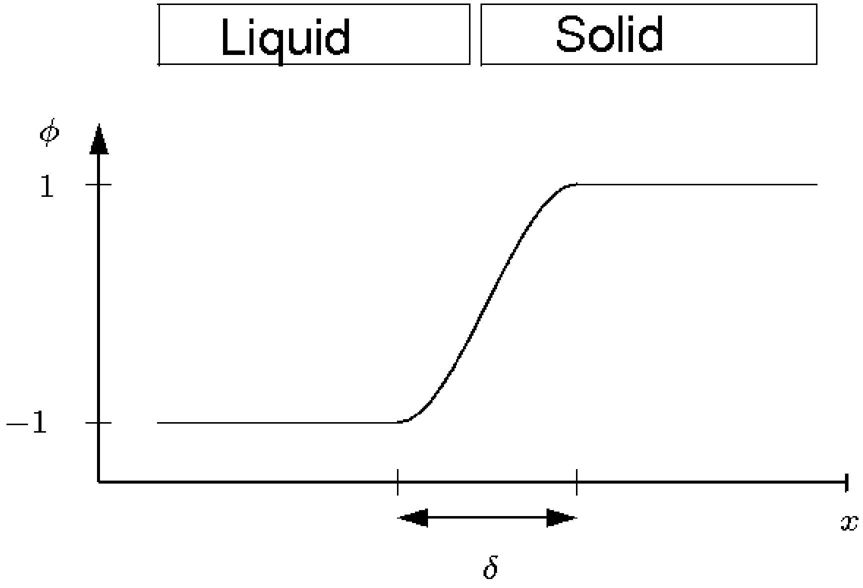
Dilute Alloys

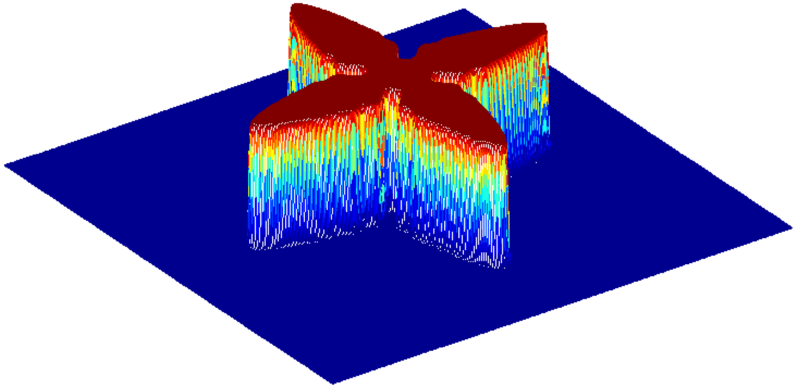
Temperature + *Concentration*

Thermal-solute phase-field model (2-d)

• Basic Idea of Phase-Field

Phase-field variable describes microstructure
with diffuse interface approach





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Thermal-solute phase-field model (2-d)

• Karma's Phase-field model

$$A(\psi)^2\left[\frac{1}{Le}+Mc_\infty[1+(1-k)U]\right]\frac{\partial\phi}{\partial t}=A(\psi)^2\nabla^2\phi+2A(\psi)A'(\psi)\left[\frac{\partial\psi}{\partial x}\frac{\partial\phi}{\partial x}+\frac{\partial\psi}{\partial y}\frac{\partial\phi}{\partial y}\right]$$
$$-\frac{\partial}{\partial x}\left(A(\psi)A'(\psi)\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial y}\left(A(\psi)A'(\psi)\frac{\partial\phi}{\partial x}\right)+$$
$$\phi-\phi^3-\lambda(1-\phi^2)^2(\theta+Mc_\infty U)$$

Phase Equation

Properties:

- highly nonlinear
- noise introduced by anisotropy function A(Ψ)
- where $\psi=\arctan(\phi_y/\phi_x)$

Thermal-solute phase-field model (2-d)

• Karma's Phase-field Model

$$
\left(\frac{1+k}{2}-\frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t}=D\left(-\frac{1}{2}\left[\frac{\partial \phi}{\partial x}\frac{\partial U}{\partial x}+\frac{\partial \phi}{\partial y}\frac{\partial U}{\partial y}\right]+\frac{1-\phi}{2}\nabla^2 U\right)+
$$

$$
\frac{1}{2\sqrt{2}}\left(\{1+(1-k)U\}\left(\frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial t}\frac{\phi_x}{|\nabla \phi|}\right)+\frac{\partial}{\partial y}\left(\frac{\partial \phi}{\partial t}\frac{\phi_y}{|\nabla \phi|}\right)\right)\right.
$$

$$
\left.+(1-k)\left(\frac{\partial U}{\partial x}\left(\frac{\partial \phi}{\partial t}\frac{\phi_x}{|\nabla \phi|}\right)+\frac{\partial U}{\partial y}\left(\frac{\partial \phi}{\partial t}\frac{\phi_y}{|\nabla \phi|}\right)\right)\right)
$$

$$
+\frac{1}{2}\left((1+(1-k)U)\frac{\partial \phi}{\partial t}\right)
$$

Concentration Equation

Temperature Equation

$$
\frac{\partial \theta}{\partial t}=\alpha\nabla^2\theta+\frac{1}{2}\frac{\partial \phi}{\partial t}
$$

▪ highly nonlinear

Thermal-solute phase-field model (2-d)

- Karma’s Phase-field Model (multiple time scales)

$$\left(\frac{1+k}{2}-\frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t}=D\left(-\frac{1}{2}\left[\frac{\partial\phi}{\partial x}\frac{\partial U}{\partial x}+\frac{\partial\phi}{\partial y}\frac{\partial U}{\partial y}\right]+\frac{1-\phi}{2}\nabla^2 U\right)+$$

$$\frac{1}{2\sqrt{2}}\left(\{1+(1-k)U\}\left(\frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial t}\frac{\phi_x}{|\nabla\phi|}\right)+\frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial t}\frac{\phi_y}{|\nabla\phi|}\right)\right)\right.$$

$$\left.+(1-k)\left(\frac{\partial U}{\partial x}\left(\frac{\partial\phi}{\partial t}\frac{\phi_x}{|\nabla\phi|}\right)+\frac{\partial U}{\partial y}\left(\frac{\partial\phi}{\partial t}\frac{\phi_y}{|\nabla\phi|}\right)\right)\right)$$

$$+\frac{1}{2}\left((1+(1-k)U)\frac{\partial\phi}{\partial t}\right)$$

D

Concentration Equation

α

Temperature Equation

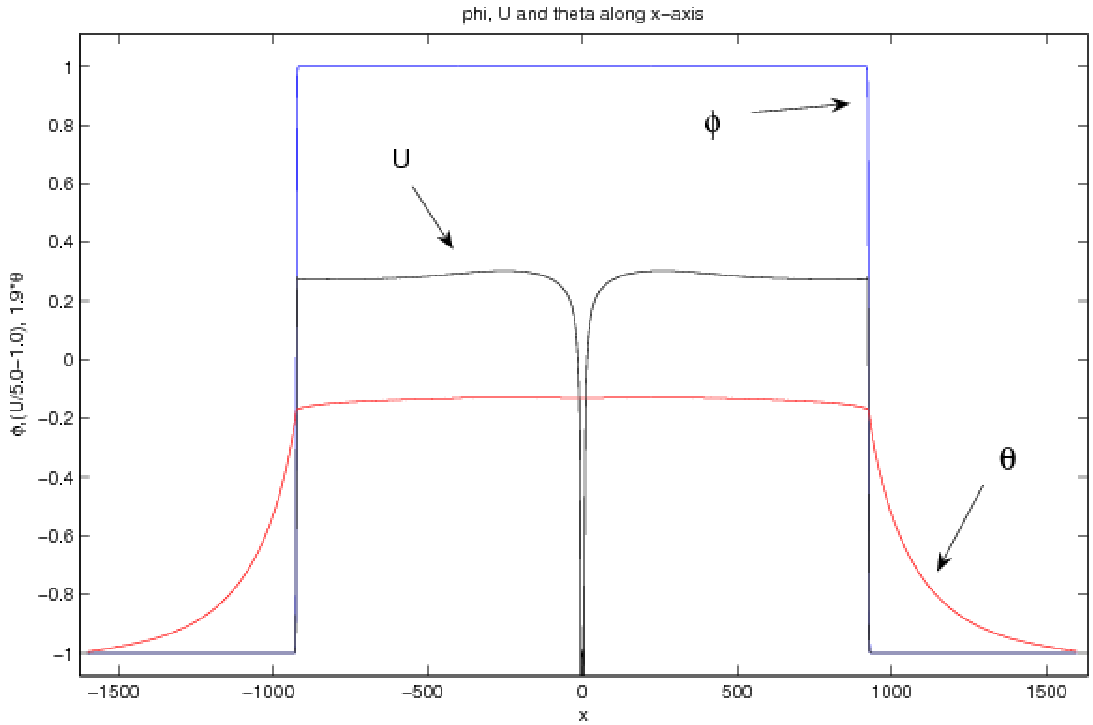
$$\frac{\partial\theta}{\partial t}=\alpha\nabla^2\theta+\frac{1}{2}\frac{\partial\phi}{\partial t}$$

- highly nonlinear

Thermal-solute phase-field model (2-d)

• Multiscale Problem

Cross-section of typical solution



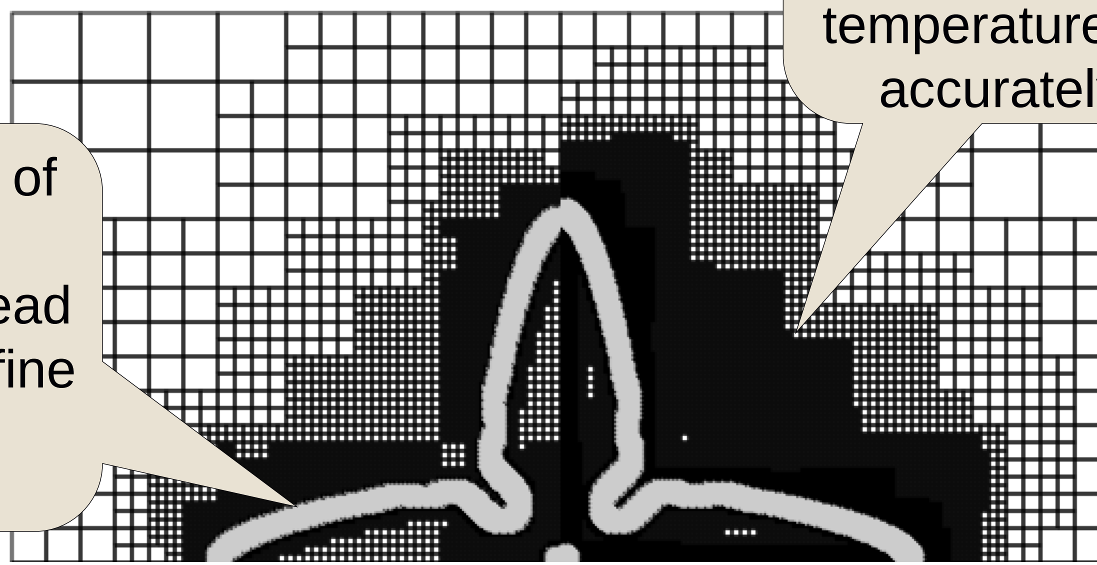
Large ratios of the diffusion coefficients lead to a multiscale problem that is highly stiff

Adaptive spatial discretization

• Adaptive mesh refinement

- Based upon quadrilateral meshes (non-uniform)
- Have implemented serendipity finite elements (p=1,2,3)
- Also implemented <u>FD stencils (2nd order used here)</u>
- Adaptive remeshing is controlled by a gradient criterion

Further mesh refinement on coarser levels to represent the temperature field accurately !!



The sharp interfaces of the phase and concentration fields lead to large gradients so fine mesh resolution is essential !!

Implicit temporal discretization

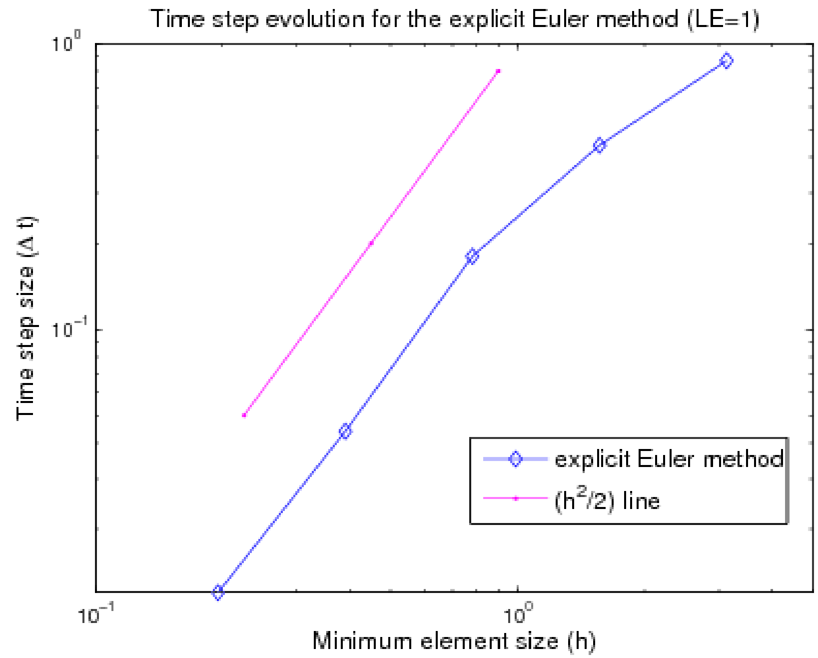
• Explicit time integration methods

- Explicit methods are "easy" to apply

  but impose a time step restriction

$$\Delta t = C \frac{h^2}{2}$$

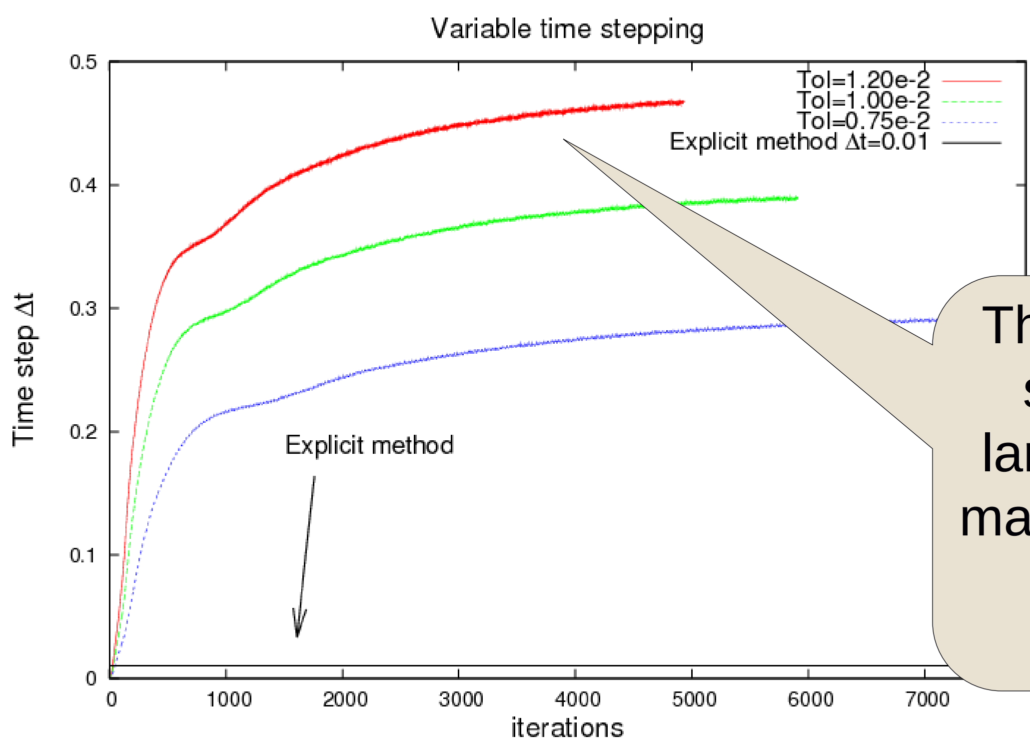
  - Very fine mesh resolution is needed to resolve the large gradients in the interface region, so the time steps become **excessively** small (not viable).



Implicit temporal discretisation

• Adaptive time step control

• **Fully implicit** BDF2 method, combined with ***variable time stepping*** (based upon a local error estimator), is used to overcome time-step restrictions...

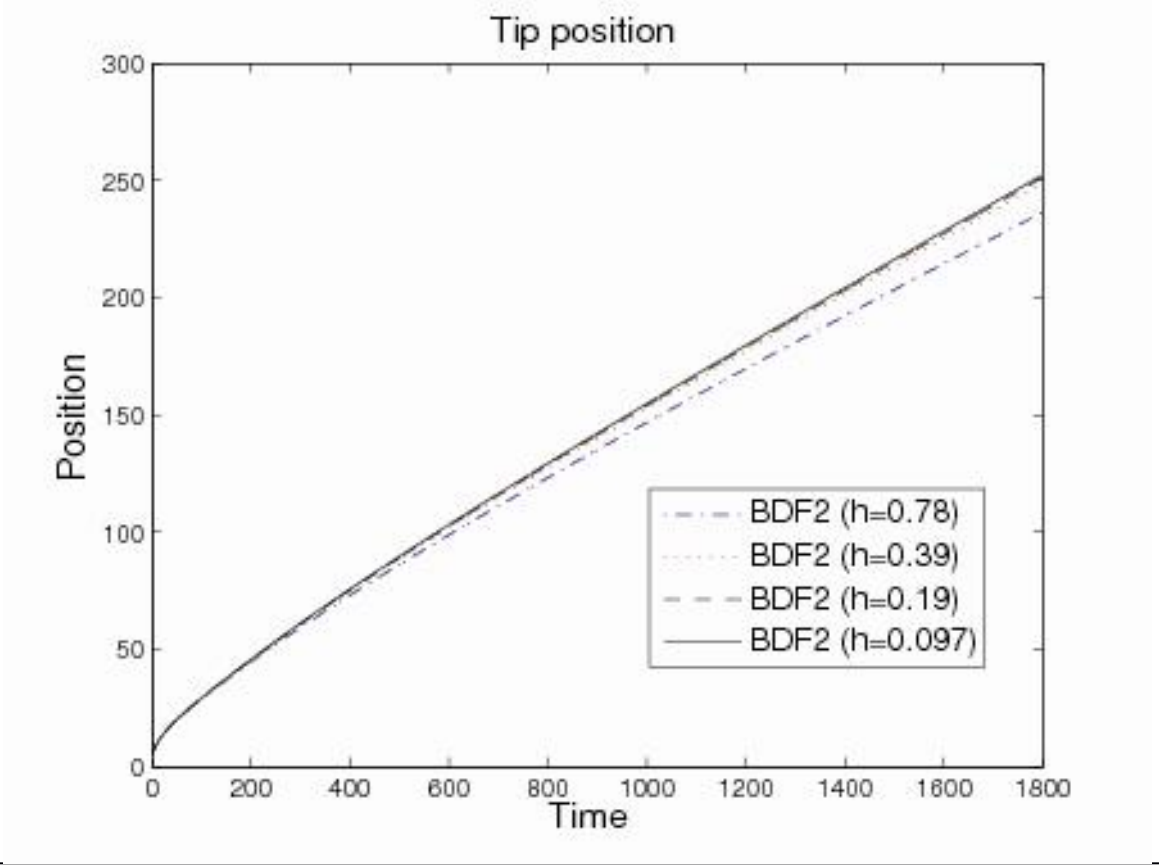


The adaption of the time step leads to a much larger time step than the maximum stable time step for the explicit Euler method !!

Implicit temporal discretisation

• Convergence of solution as maximum mesh level is increased

• The BDF2 method allows sufficiently fine spatial meshes to be used:



Nonlinear multigrid solver

• Nonlinear multigrid solver for adaptive meshes

At each time step a large nonlinear algebraic system of equations must be solved for the new values: ϕ_{ij}^{n+1}, U_{ij}^{n+1} and θ_{ij}^{n+1}.

Unless this can be done efficiently the method is worthless…

- A f*ully coupled* nonlinear Multigrid solver is used to achieve this:
    - ➢ based upon the FAS (full approximation scheme) approach to resolve the non-linearity
    - ➢ and the MultiLevel AdapTive (MLAT) scheme of Brandt to handle the adaptivity
    - ➢ a pointwise weighted nonlinear Gauss-Seidel iterative scheme is seen to be an adequate smoother.
- Excellent, *h*-independent, convergence results are obtained.

Nonlinear multigrid solver

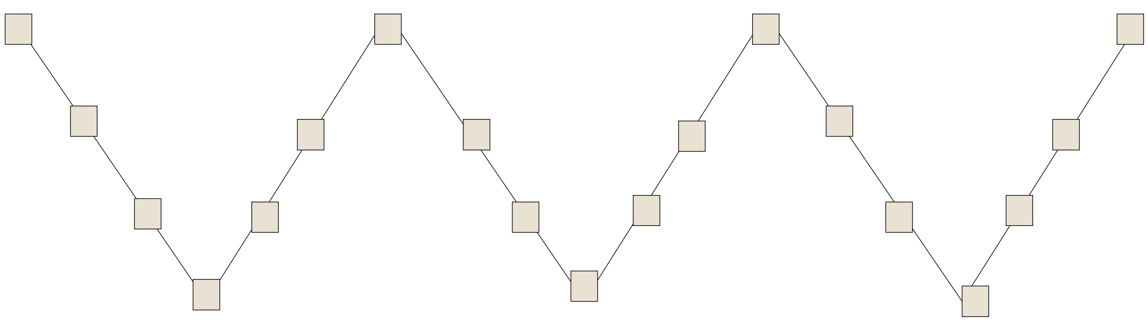
• The FAS scheme

The FAS scheme, for solving A(U)=f, has the following features…

•Smoother is nonlinear -- we use a pointwise weighted G-S scheme:

$$u_{ij}^{k+1} = u_{ij}^{k+1} - \omega \frac{(A(u_{ij}^{k+1}) - f_j)}{\partial A / \partial u_{ij} \, (u_{ij}^{k+1})}$$

•Based upon a standard V-cycle at each time step:



Nonlinear multigrid solver

• The FAS scheme

- In this implementation:
  - Interpolation from coarse to fine grids is *bilinear*
  - Restriction from fine to coarse grids is simple *injection*

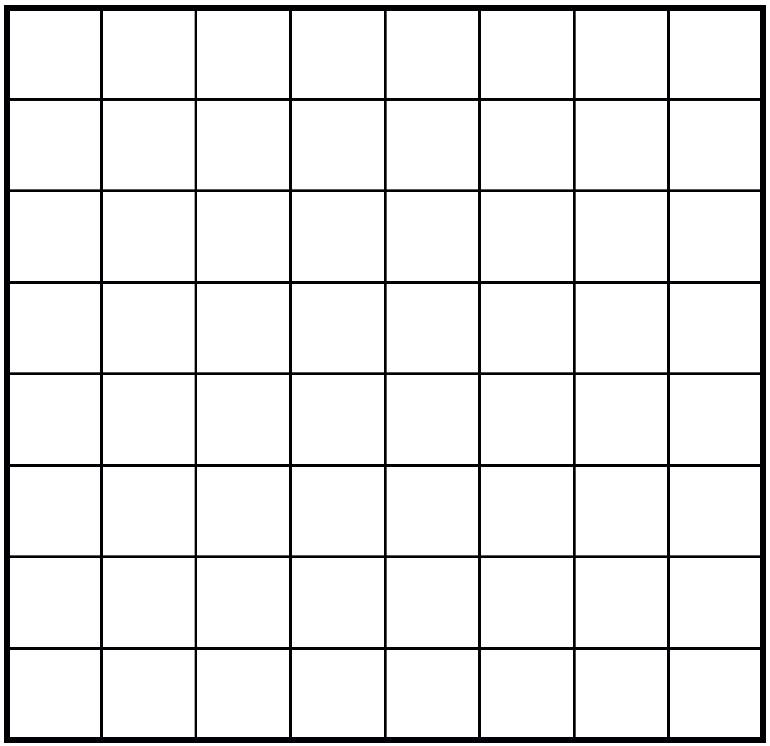
- The correction step requires an approximation to the full coarse grid problem but with a modified right-hand-side:

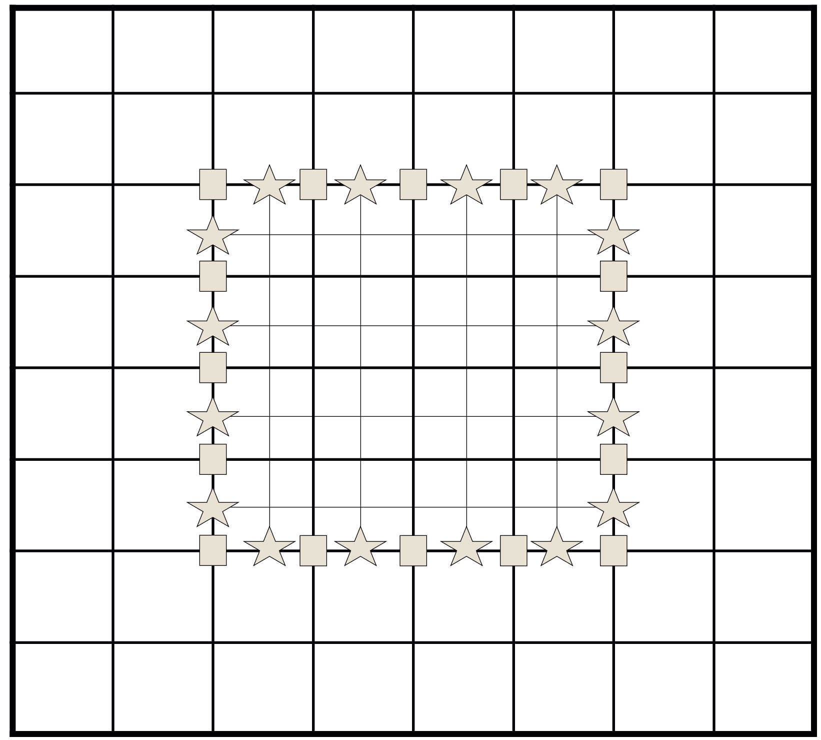
$$f_{2h} = I_h^{2h}(f_h - A_h(u_h)) + A_{2h}(I_h^{2h}u_h)$$

Nonlinear multigrid solver

• The MLAT scheme

For the MLAT scheme the nodes at the interface between refinement levels are treated as a Dirichlet boundary by the smoother…

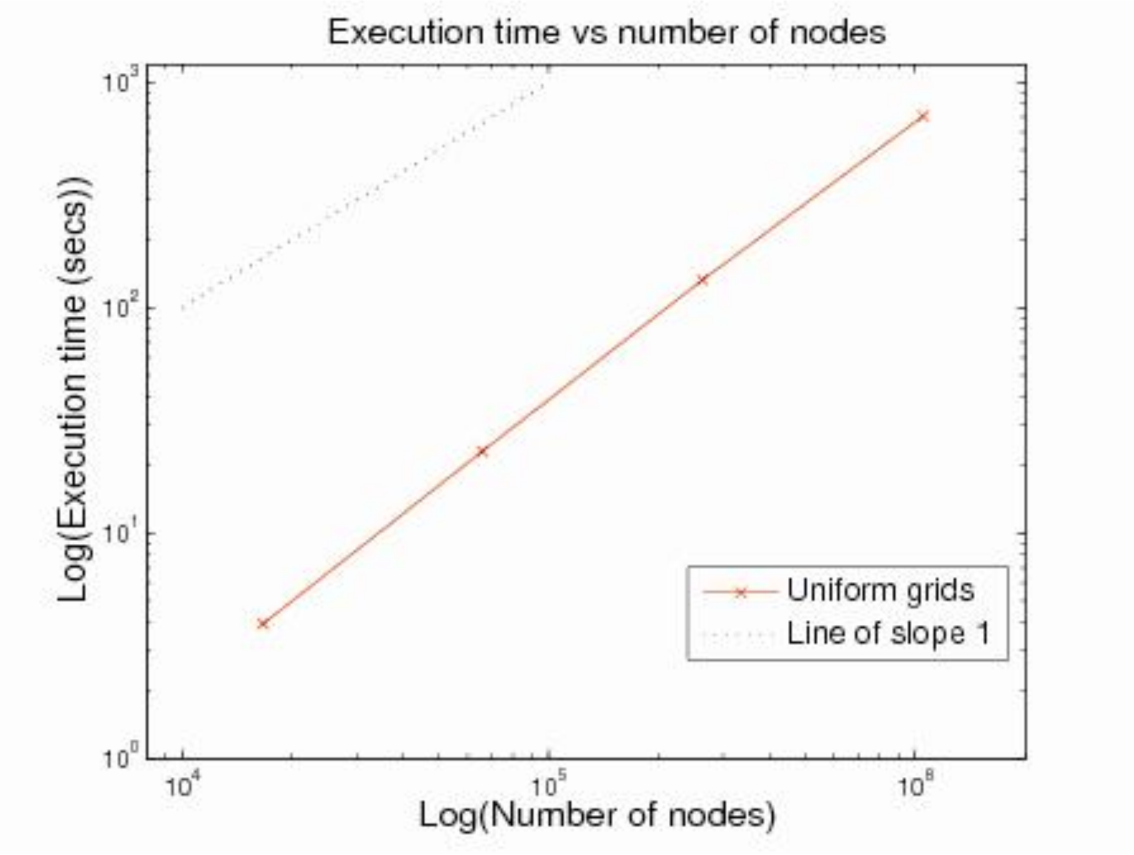




Nonlinear multigrid solver

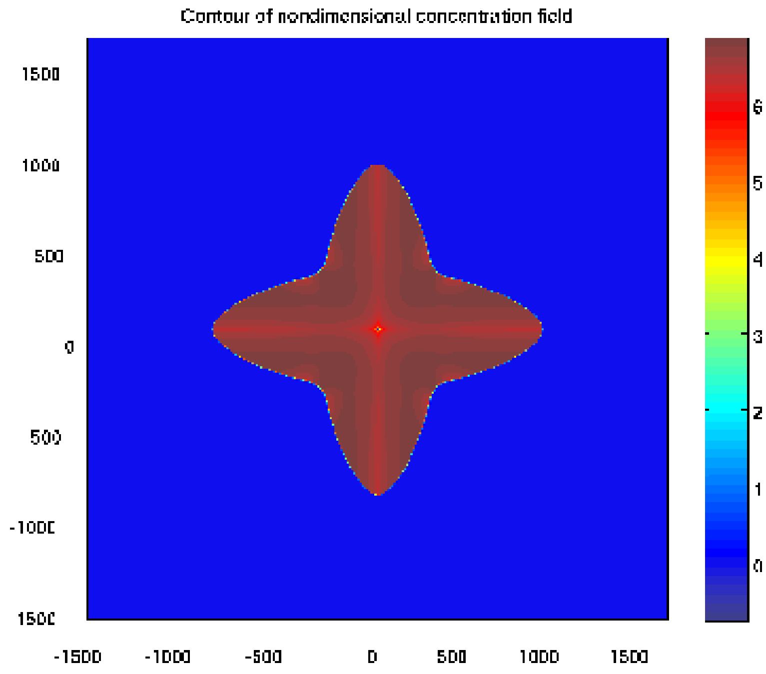
- Nonlinear multigrid solver for adaptive meshes

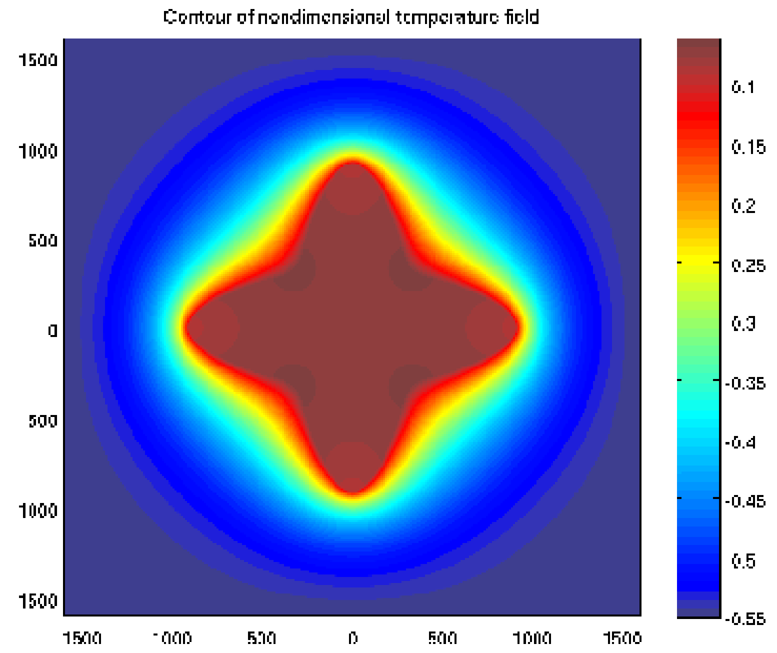
- Here we see the optimal solution time for the nonlinear multigrid solver:



Results in 2-d

- Dilute binary alloy solidification simulation with Lewis number 500

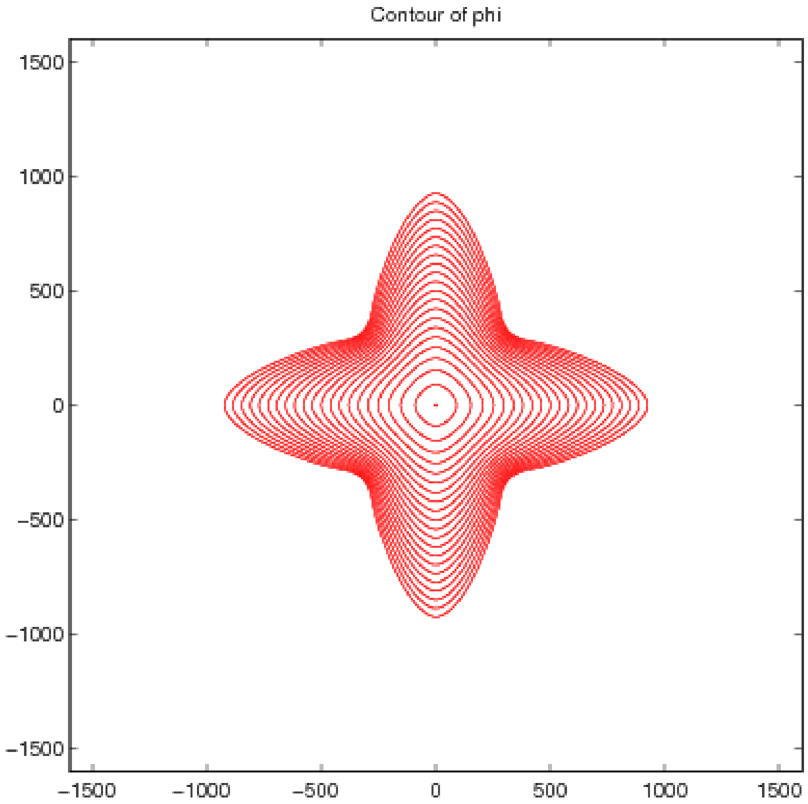


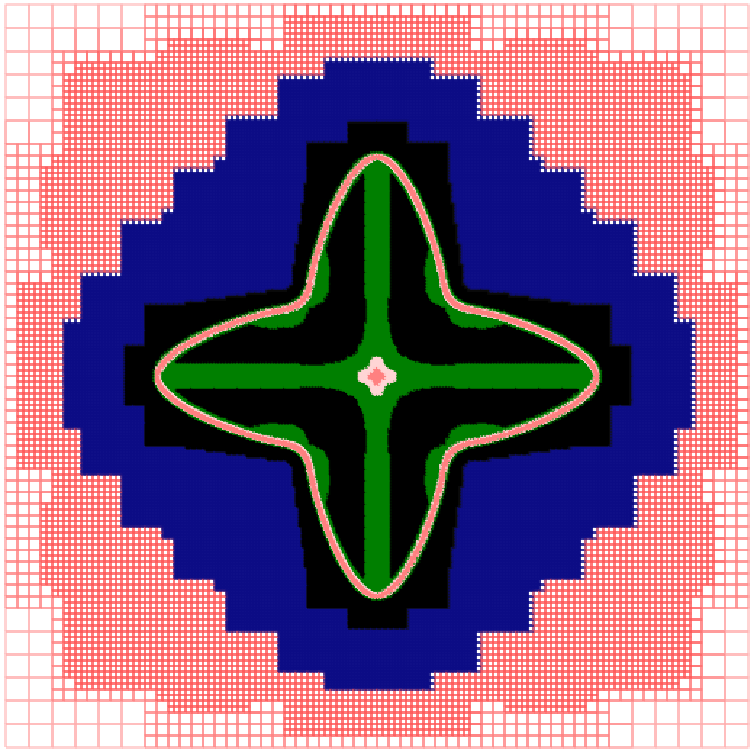


Lewis number 500

Results in 2-d

- Progression of the adaptive mesh





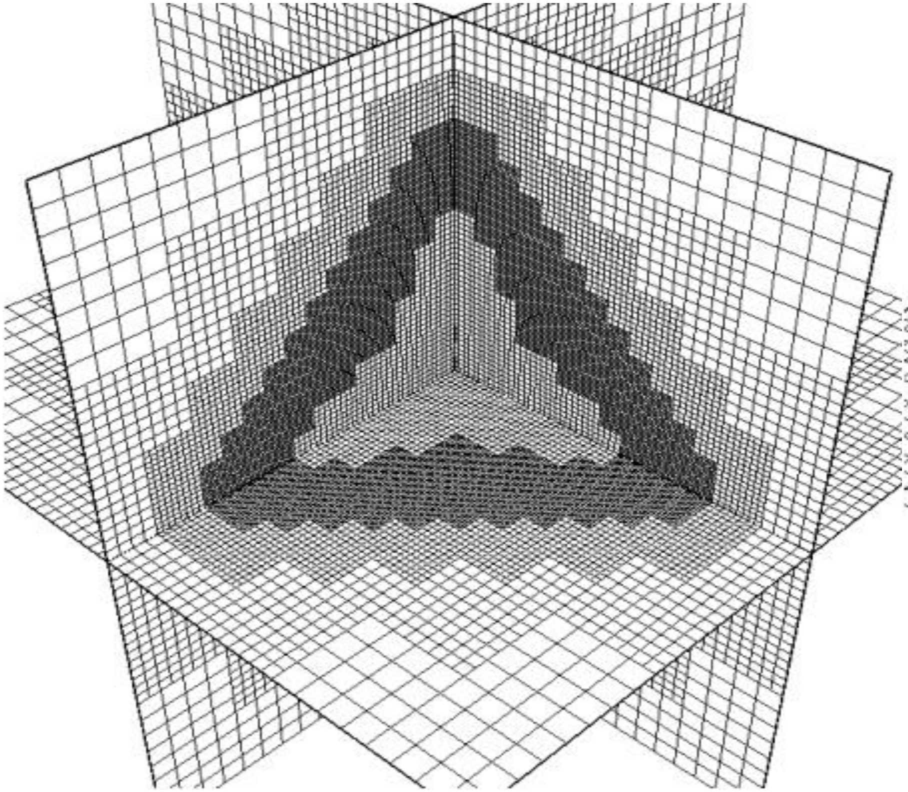
Parallel implementation in 3-d

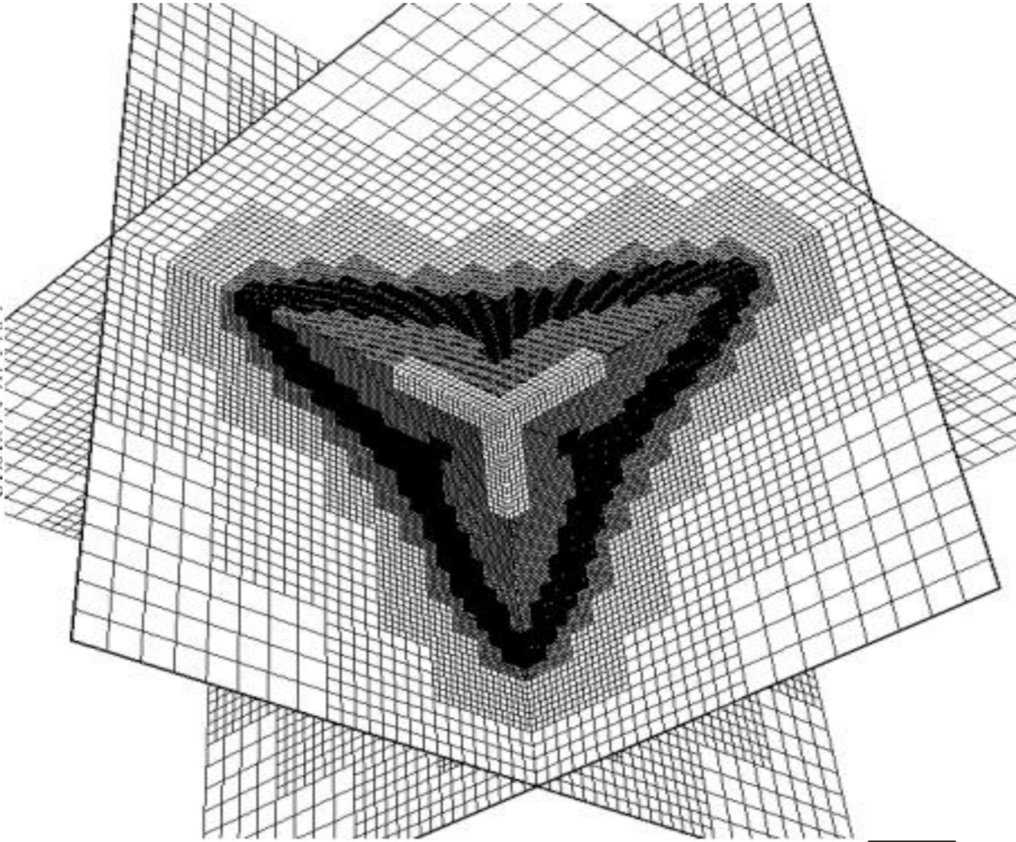
- Initial development for models of a (i) a pure melt, or (ii) isothermal alloy:
  - ➢equations generalize naturally to three dimensions,
  - ➢extension to fully coupled model discussed at the end.
- The solution approach also generalises naturally to 3-d:
  - ➢adaptivity on hexahedral meshes,
  - ➢fully implicit time-stepping with 3-d nonlinear multigrid.
- Unlike in 2-d it is not feasible to solve on a workstation – need to make use of parallel computing:
  - ➢impossible to get required level of refinement without this,
  - ➢cannot use parallelism instead of adaptivity and multigrid – it must be used *in addition* to these!

Parallel implementation in 3-d

• Adaptivity

• Examples of 3-d adaptivity with different refinement levels…





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Parallel implementation in 3-d

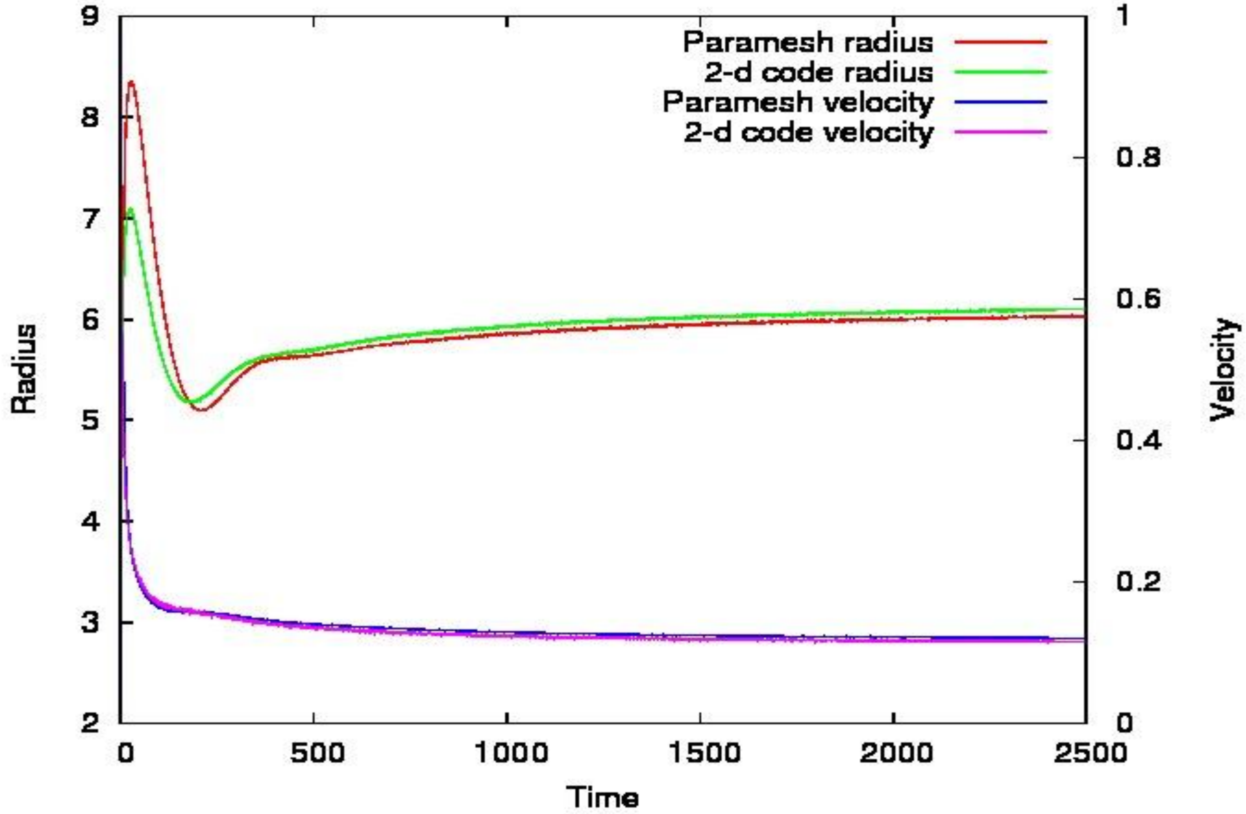
- The use of PARAMESH

- The previous meshes were obtained using PARAMESH:
  - an open source s/w library for adaptivity in parallel,
  - uses hierarchical refinement and derefinement of blocks,
  - guard cells ensure that the programmer need not be concerned about data location when implementing their discretization scheme,
  - we use a cell-centred finite difference approach for convenience.
- We have made numerous modifications to this library:
  - implementation of the FAS multigrid scheme to support the solution of our nonlinear systems at each time step,
  - necessary modifications to support the MLAT scheme using the adaptive data structures.

Parallel implementation in 3-d

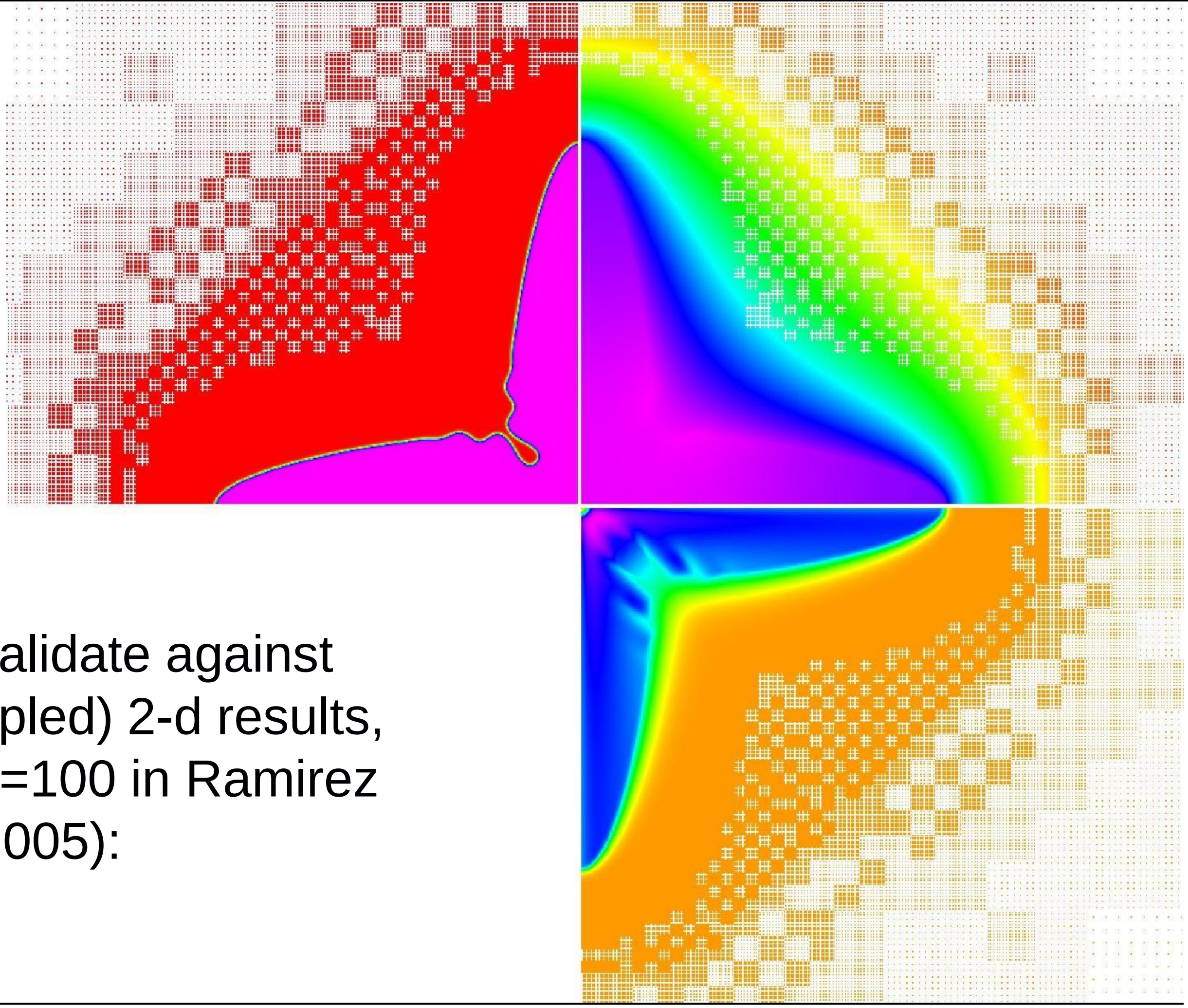
• The use of PARAMESH

• We validate the PARAMESH implementation by restricting to 2-d and making a comparison against our existing (fully-coupled) 2-d results:



Parallel implementation in 3-d

• The use of PARAMESH

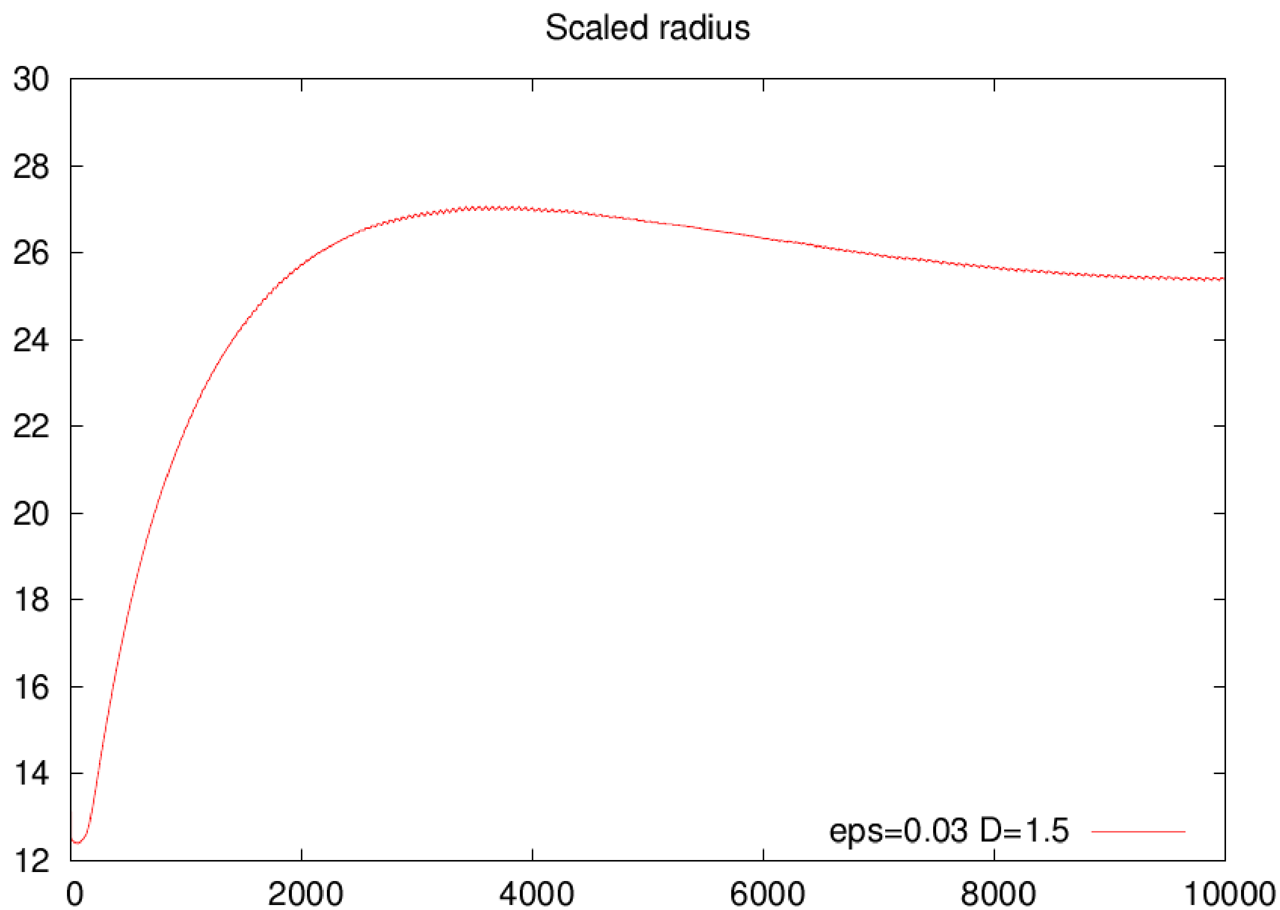


• Similarly we can validate against published (fully-coupled) 2-d results, such as those at Le=100 in Ramirez and Beckermann (2005):

Parallel results in 3-d

- For a model of a pure melt (thermal and phase fields only)

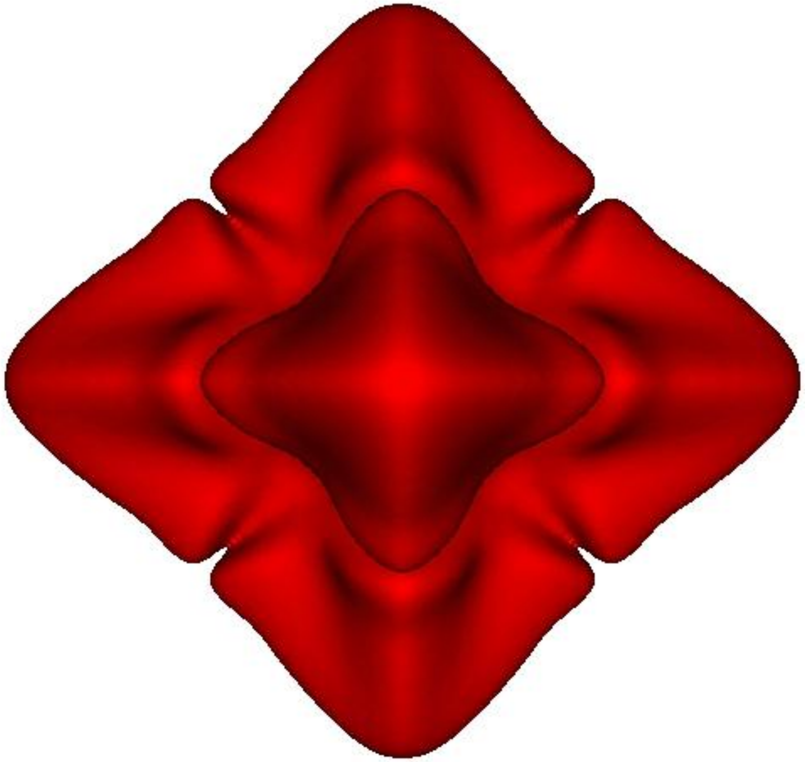
- Successful validation against the 3-d *thermal only* results of Karma and Rappel (1998) et al.…
- The graph of the tip radius tends to the same steady-state value
- Similar match for tip velocity.



Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

- An example of solidification with a six-fold symmetry…

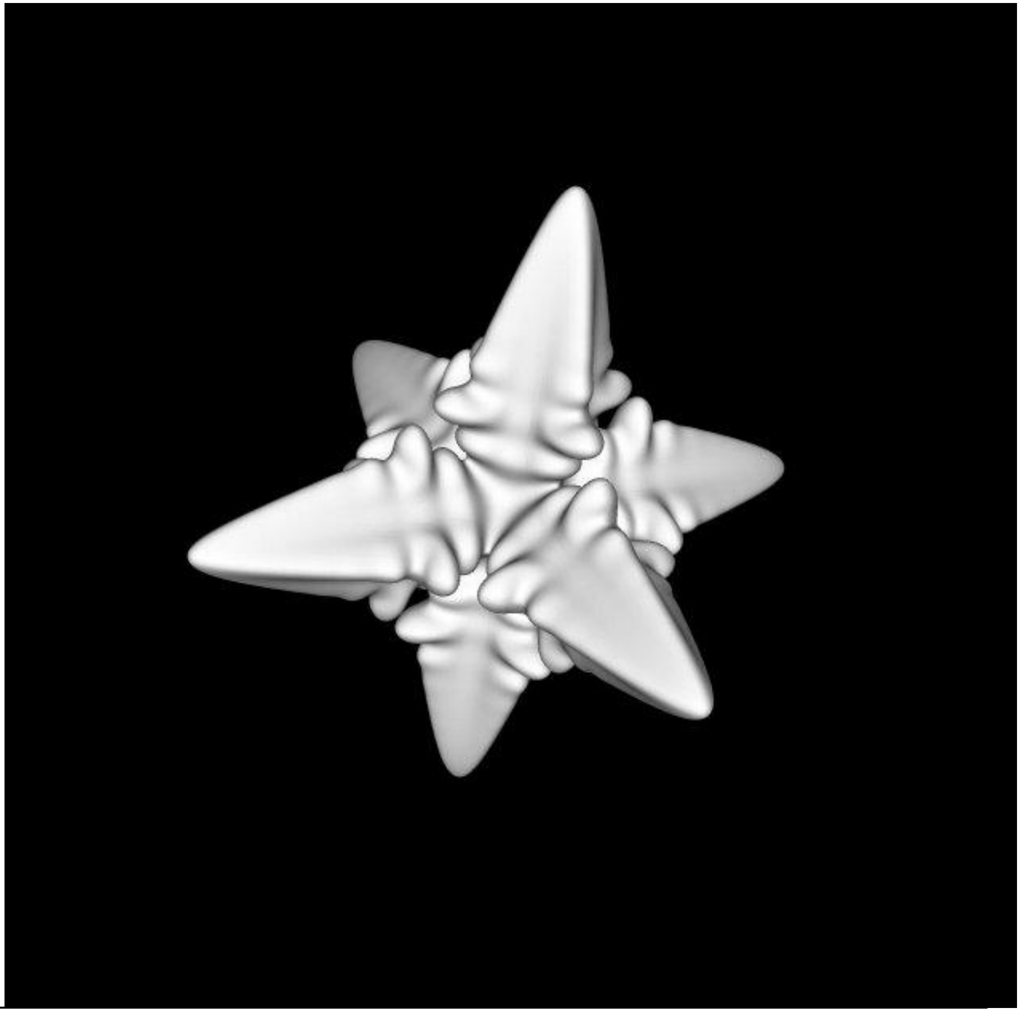


Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

•A snap shot of a different 3-d dendrite.

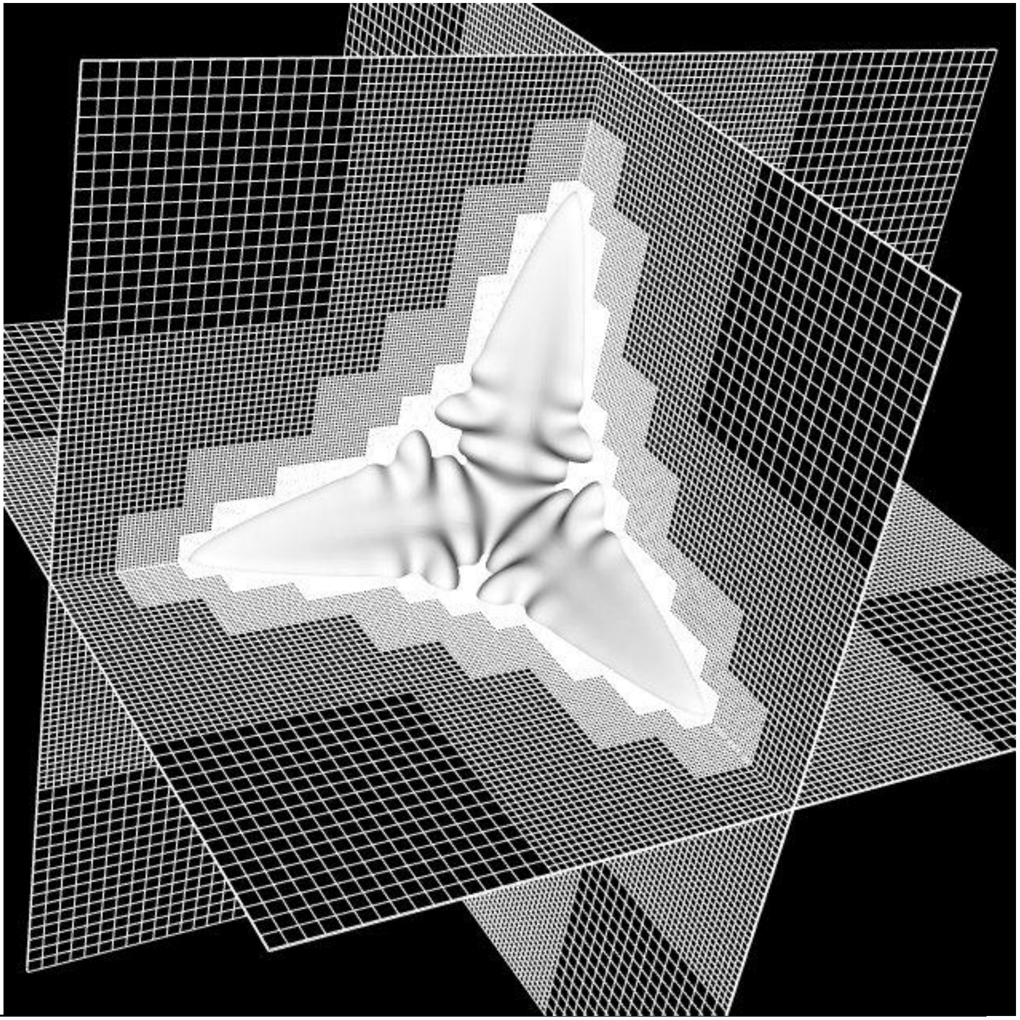
•This image shows the single isosurface Φ=0….



Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

- A snap shot of the same 3-d dendrite as in the previous slide.
- This image shows the isosurface along with the adapted mesh…

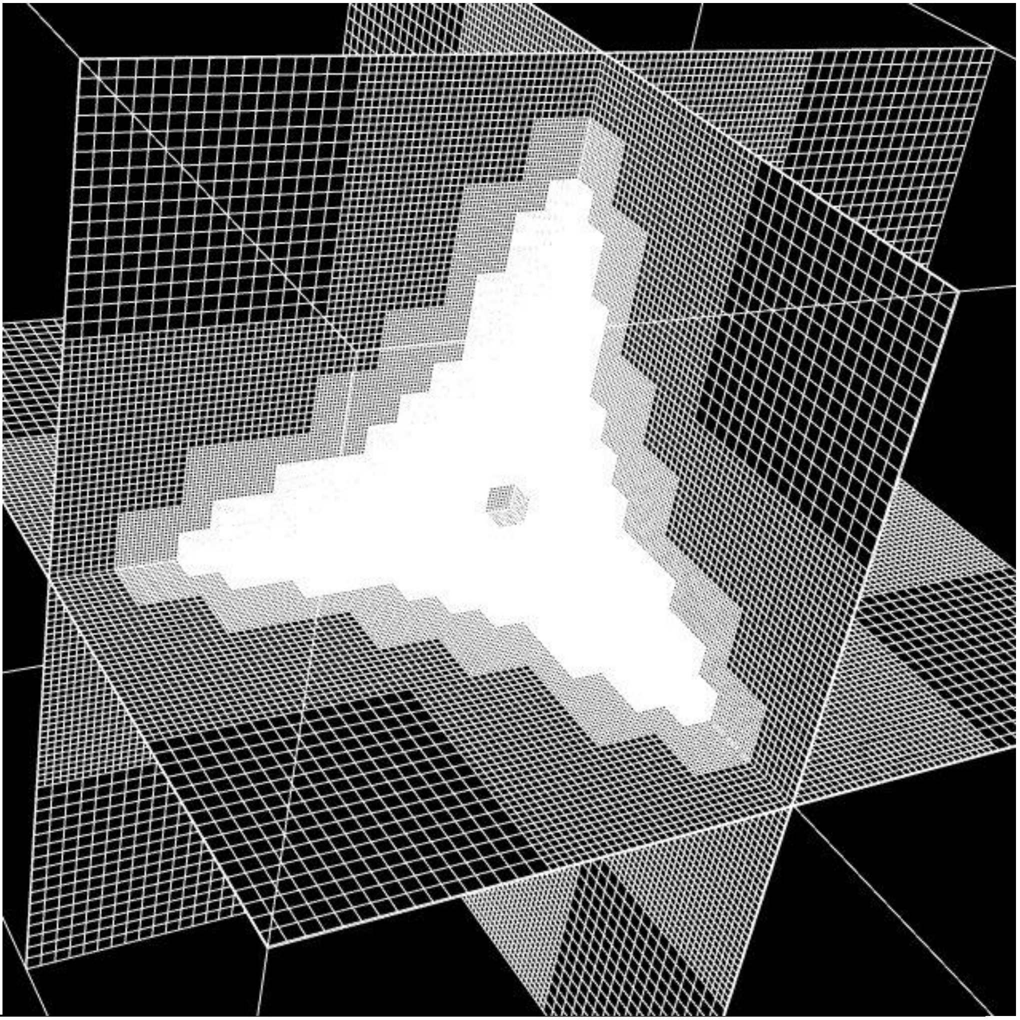


Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

•A snap shot of the same 3-d dendrite again.

•This image shows only the adapted mesh…



Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

- Some parallel performance results using a fixed problem size…
  - ➢ Uniformly refined mesh.
  - ➢ Rather small problem (just over two million cells).
  - ➢ Speed-up and Efficiency shown relative to 8 core case.

Cores	Time (s)	Speed-Up	Efficiency
8	6611		
16	4298	1.54	77%
32	2796	2.36	59%
64	1734	3.81	48%

Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

- The fixed problem size is not very realistic…
  - ➢ Aim of parallelism here is to allow larger problems to be solved.
  - ➢ We now show a sequence of finer and finer grids.
  - ➢ Again uniform mesh refinement is assumed.

Cores	Cell count	Time (Time per V-cycle)	Efficiency
1	262k	1453 (27.9)	
8	2,097k	1577 (20.5)	136%
64	16,777k	3717 (30.5)	91%

Parallel results in 3-d

• For a model of a pure melt (thermal and phase fields only)

• Justification for requiring both parallelism and adaptivity…

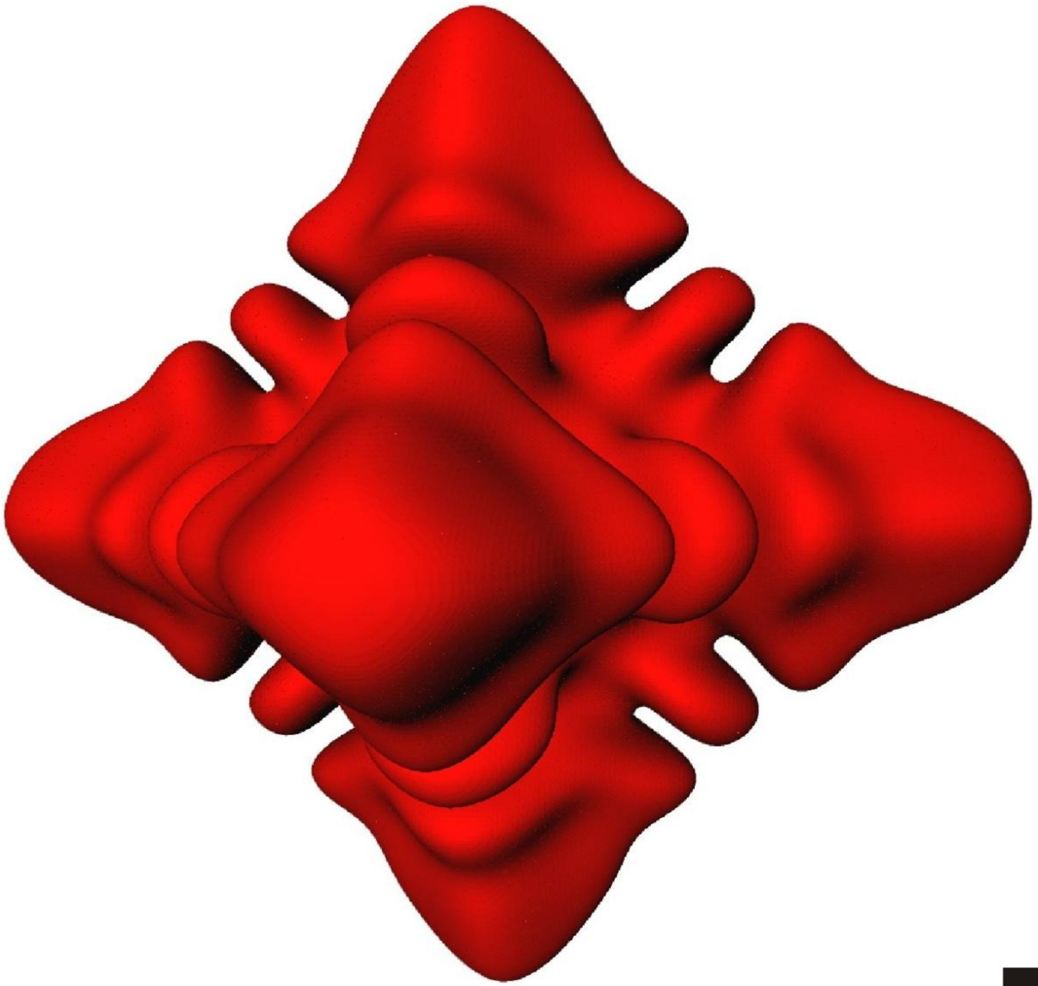
Cores	Uniform Grid Level (Cells)	Adapted Grid Level (Equiv Cells)
1	7 (262k)	8 (2.1M)
2		9 (16.8M)
8	8 (2 097k)	10 (134.2M)
20		11 (1073.7M)
64	9 (16.8M)	
128		12 (8.59B)

• This is for a typical sample problem and will vary for different cases…

Parallel results in 3-d

• For a model of an isothermal binary alloy (solute and phase fields only)

- An example of solidification with a six-fold symmetry for an isothermal binary alloy…
- We have been able to successfully validate against an existing explicit solver (Danzig) – though only for relatively coarse spatial grids:
    - Tip radius
    - Tip velocity



Discussion

Numerical methods:

1. Second order finite differences for the spatial discretization of the highly nonlinear coupled system of parabolic PDEs.
2. Hierarchical adaptivity to refine and coarsen the spatial mesh as the solution evolves in time.
3. Fully implicit second order BDF time integration for the stiff ODE systems that arise after spatial discretization of high Lewis number problems.
4. Fully coupled nonlinear Multigrid solver for the nonlinear algebraic systems that occur at each time step.
5. Adaptive time step selection based upon local error estimation
6. Parallel implementation to allow progress to three space dimensions.

Discussion (cont)

2D Results:

1. First time a multiscale Phase-field solidification model has been solved fully implicitly.
2. Has allowed 2-d simulation at physically realistic Lewis number (up to 10000) for the first time (previous limit was O(100)):
   - **Physical Review E**, vol.79, 030601, 2009.
3. This enhanced capability is leading to new scientific insight - with the coupled thermal-solutal model behaving very differently from its pure solutal counterpart :
   - **J. Cryst. Growth**, vol.312, pp.1891--1897, 2010.

Discussion (cont)

3D Results:

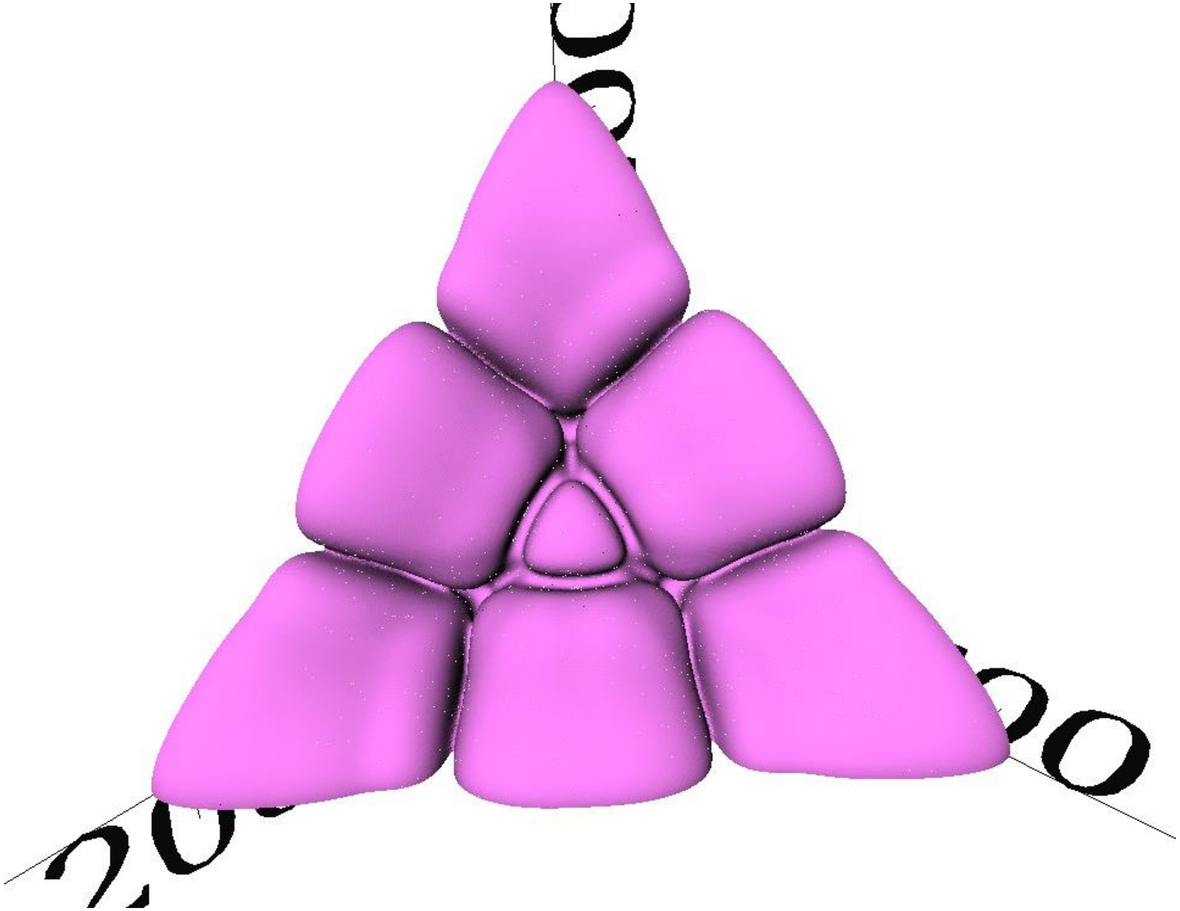
1. Parallel version essential for 3D – sequential 2D runs take many days!
2. Must retain adaptivity, implicit stiff solver & multigrid in the parallel version.
3. Implemented via the PARAMESH library...
   - Able to validate parallel version against the fully-coupled 2D code;
   - Able to validate against pure thermal 3D results:

     Numerical Methods for PDEs, vol.27, pp.106--120, 2011.
   - Also able to validate against pure solutal 3D results.
4. Now starting to produce fully-coupled 3D results for the first time...
   - Even for runs at moderate Lewis number each simulation is highly computationally expensive.

Discussion (cont.)

• Fully-coupled example in 3D

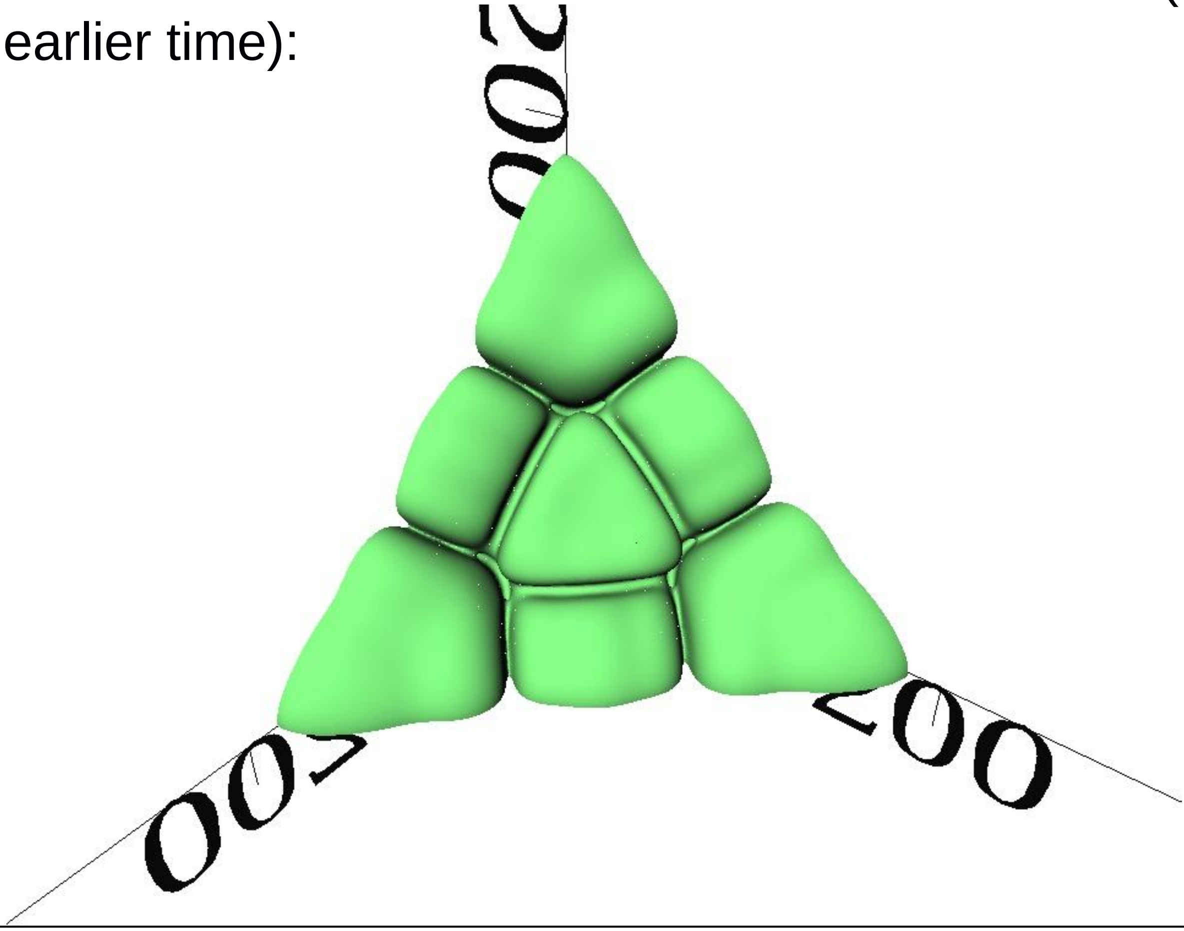
• Snapshot of the start of dendrite formulation at Le = 40:



Discussion (cont.)

• Fully-coupled example in 3D

• Snapshot of the start of dendrite formulation at Le = 40 (finer grid and slightly earlier time):



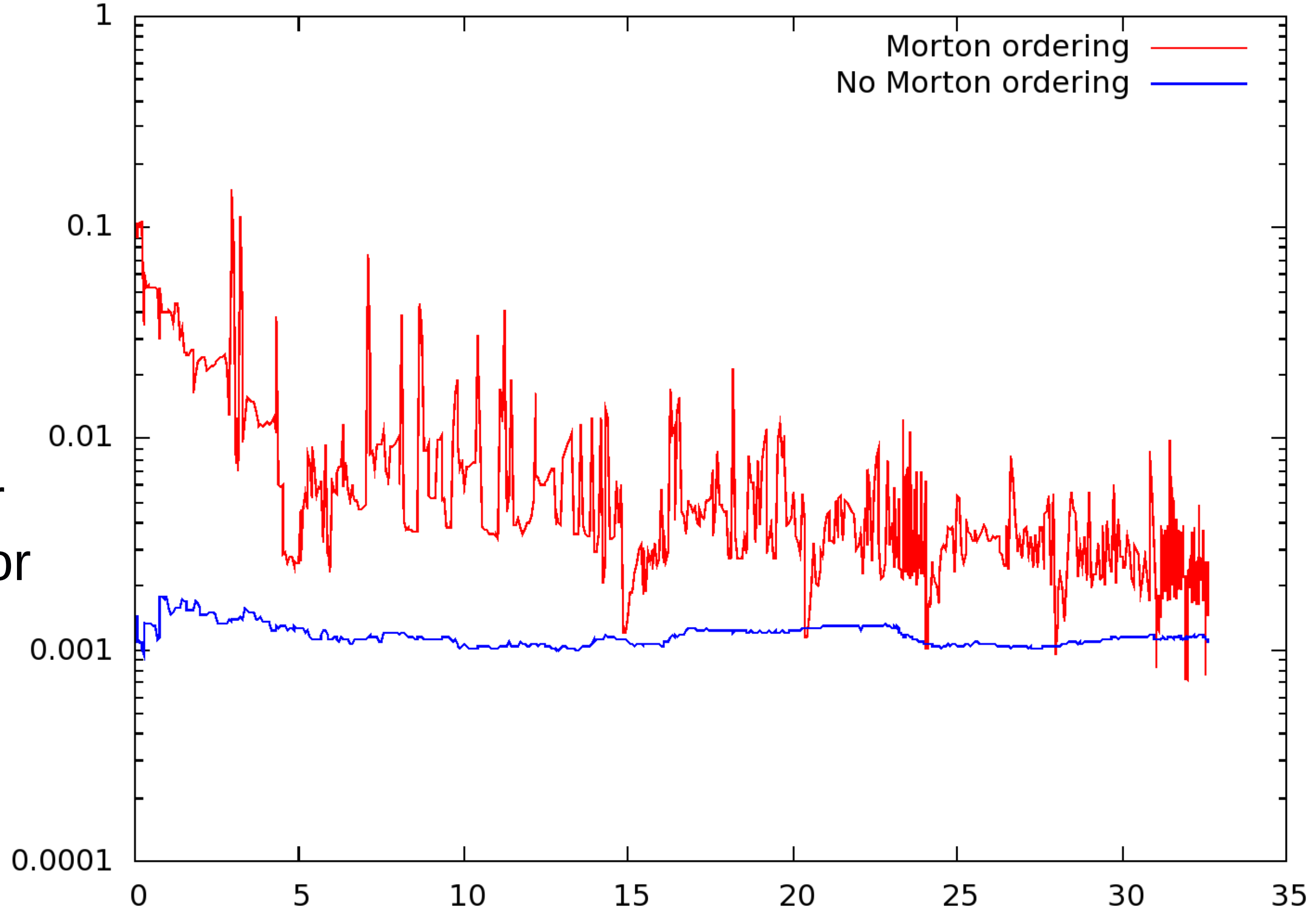
Discussion (cont)

Current work:

1. Seek to improve parallel efficiency:
    - Currently emphasis has been to provide a capability;
    - Now focusing on improving the partitioning strategy used by PARAMESH – currently based upon Morton ordering...
    - Have ported to HECToR – running on ~1024 cores.
2. Will then start to produce simulation results across a range of Lewis numbers.
3. May also consider alternative multigrid approaches:
    - Could perform a quasi-Newton linearization at each time step and then use a linear MG solver;
    - Would allow library software (e.g. for algebraic multigrid) to be used!

Discussion (cont.)

- Our initial attempts to improve the partitioning strategy are based upon balancing the load at each mesh level...
- This plot shows the computation time per block per time step for a typical 32 core run.



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