Cloud and Aerosol Research on Massively-parallel Architectures (CARMA)

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What you're about to hear

- The dCSE project
- The LEM code
- Name that cloud!
- Some "interesting science"
  - Or how this project could save the world!
- The Parallel Iterative Solver
- Testing, optimisation and future work.

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CARMA

- 12 month dCSE project with Dr Paul Connolly of Manchester University and Dr Alan Gadian of Leeds University.
  - Thanks also to Alan for the slides on the VOCALS project!
- Three main objectives
  - To implement a parallel iterative pressure solver within the LEM (Large Eddy Model) code
  - To update the existing LEM code to use FFT libraries
  - To parallelise the code ACPIM for use on HECToR

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The Aerosol-Cloud-Precipitation Interaction Model (ACPIM)

- Developed and validated at the UoM and the Institute of Meteorology and Climate Reseach in Germany
- A detailed process-scale model for studying the growth and evolution of cloud from aerosols
  - Will be used to test our ability to simulate ice formation on aerosols in the atmosphere

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New Science

- The parallelisation of ACPIM
  - will provide the research community with a model capable of simulating very detailed processes on cloud-scale systems, bridging the gap between laboratory work, cloud modelling and analysis of field data.

The Large Eddy Model (LEM)

- Code developed by The Met Office
- Widely used in academic research
- High resolution numerical model used to simulate cloud-scale and microscale atmospheric processes
  - e.g. aerosol-cloud interactions
  - Modified Navier-Stokes with parameterisations for turbulence, microphysical processes and radiation

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Basic Equation Set

- The LEM solves the following basic equation set, shown using tensor notation:

$$\frac{Du_i}{Dt} = -\frac{\partial}{\partial x_i}\left(\frac{p'}{\rho_s}\right) + \delta_{i3}B' + \frac{1}{\rho_s}\frac{\partial \tau_{ij}}{\partial x_j} - 2\epsilon_{ijk}\Omega_j u_k \quad (1)$$

$$\frac{\partial}{\partial x_i}(\rho_s u_i) = 0 \quad (2)$$

$$\frac{D\theta}{Dt} = \frac{1}{\rho_s}\frac{\partial h_i^\theta}{\partial x_i} + \left(\frac{\partial \theta}{\partial t}\right)_{mphys} + \left(\frac{\partial \theta}{\partial t}\right)_{rad} \quad (3)$$

$$\frac{Dq_n}{Dt} = \frac{1}{\rho_s}\frac{\partial h_i^{q_n}}{\partial x_i} - \left(\frac{\partial q_n}{\partial t}\right)_{mphys} \quad (4)$$

Parallel Iterative Pressure Solver

- Implementation of an iterative method for solving Poisson's Equation
  - Removes the need for periodic boundary conditions
  - and so extends the science that the LEM can be used for.

New Science

- With the new parallel iterative solver
  - The code could be used to study lightning generation and the electrification of clouds
    - Leading to a lightning predictor tool
  - Non-periodic solutions are needed for the multi-national VOCALS (Vamos Ocean Cloud Atmosphere Land Study) project, an investigation of stratocumulus clouds in the south-east Pacific and their effect on climate.

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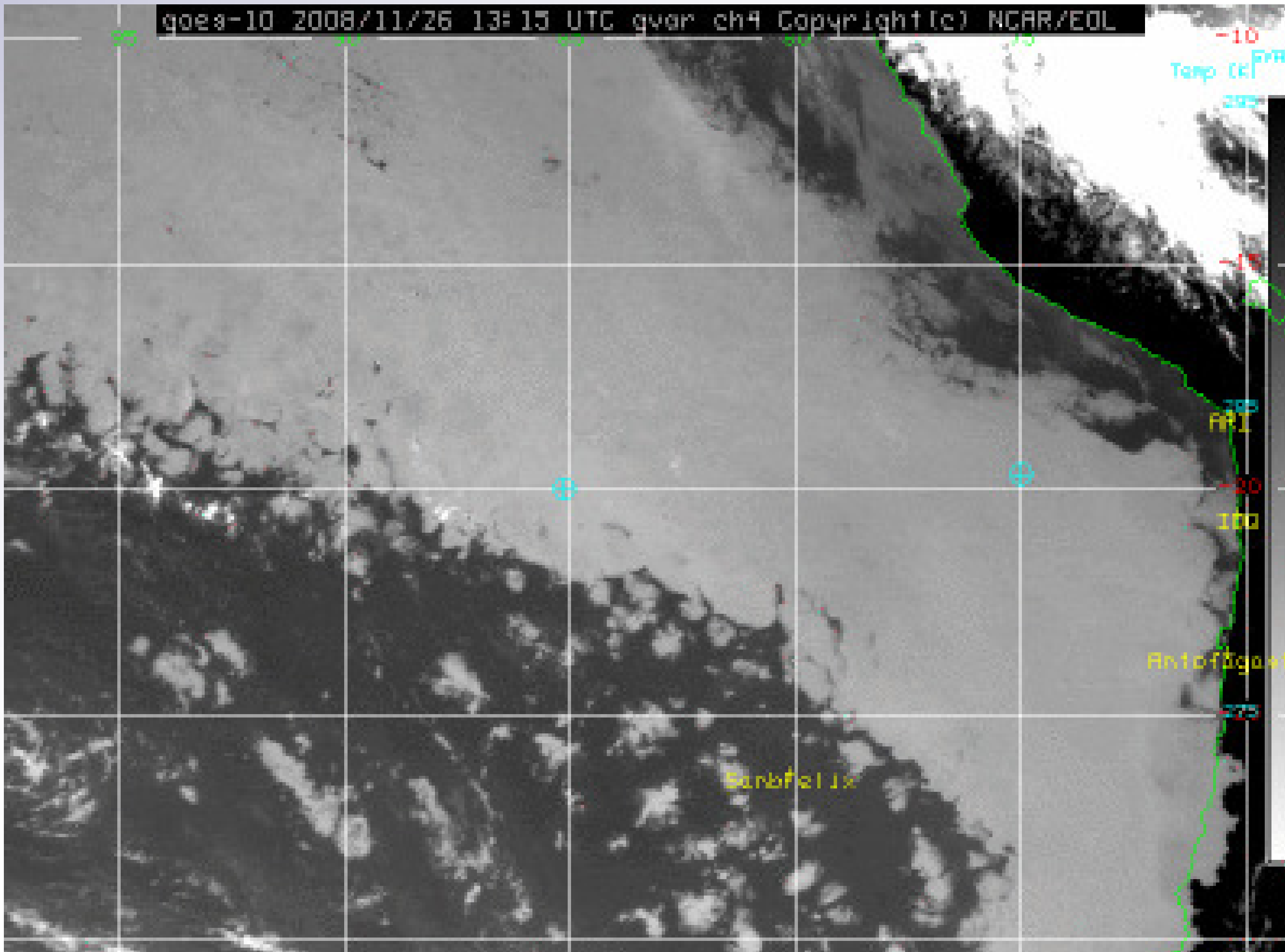
Name That Cloud!



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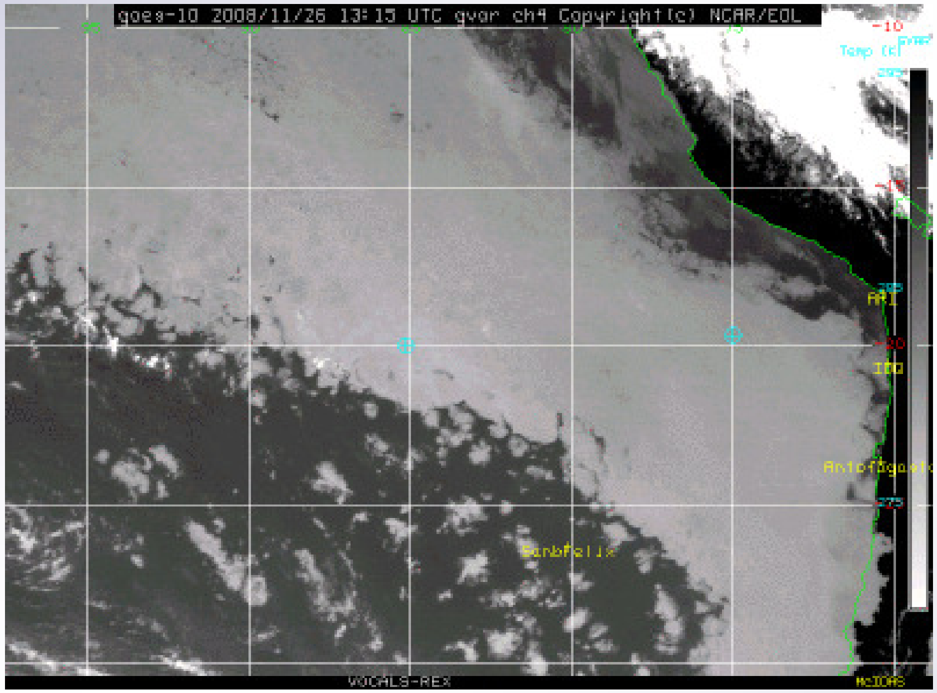
- Stratocumulus Clouds cover more than 30% of Ocean Surface
- Stratocumulus Clouds have a high reflectance, which depends on droplet number and mean droplet size.

<u>Twomey Effect</u>.

Lots of small drops, produce whiter clouds.



Smaller glass beads are whiter.

November 2008, during VOCALS. Stratocumulus clouds off the coasts of Chile and Peru (US and UK scientists)

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Technique *(Latham, Nature, 1990)*

1. Latham et al. Phil Trans of
2. Salter et al. Nov 2008.

To disseminate “natural” sea-water 0.8 micron droplets at ocean surface, into the boundary layer.

These ascend via thermals and turbulence to cloud-base levels in sufficient quantities and with sufficient salt-mass to dominate as CCN, thereby increasing N, in a quantitatively controllable manner, and mono dispersed size distribution.

Switching off the sprayers, returns to the status quo within weeks

Stephen Salter’s design, picture courtesy John McNeill

Support for idea

- Natural droplet creation at ocean surface.
- Bubble-bursting, white-capping
- NaCl droplets are effective CCN
- Ship tracks, fires, industrial pollution etc.

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Cloud Whitening

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Some LEM code details

- Mainly Fortran77 but with some Fortran90
  - All memory statically allocated
- Communication written using GCOM
  - A wrapper around a wrapper around a subset of MPI
- “Version control” using nupdate
  - Decks, comdecks and nupdate

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Running the LEM

- Jobs compiled and submitted via scripts
  - lemsub and runXT4
- Set-up jobs and chain jobs
  - Jobs can resubmit themselves, reading the input from the previous job

Decomposition of the Domain

- The domain is made up of IIP×JJP×KKP grid-points.
- Integration of the equations only requires information from up to 2 grid-points away so the domain can be decomposed into sub-domains with overlapping halo regions.
- A centred-difference time integration scheme is used.

Decomposition of the Domain

- The LEM integrates the field in a succession of 2D slices in the y-z plane, moving along the x-direction.
- The domain is decomposed in the x-direction so that each PE holds IIP/NPES slices, along with a two-slice halo region for each neighbouring sub-domain.

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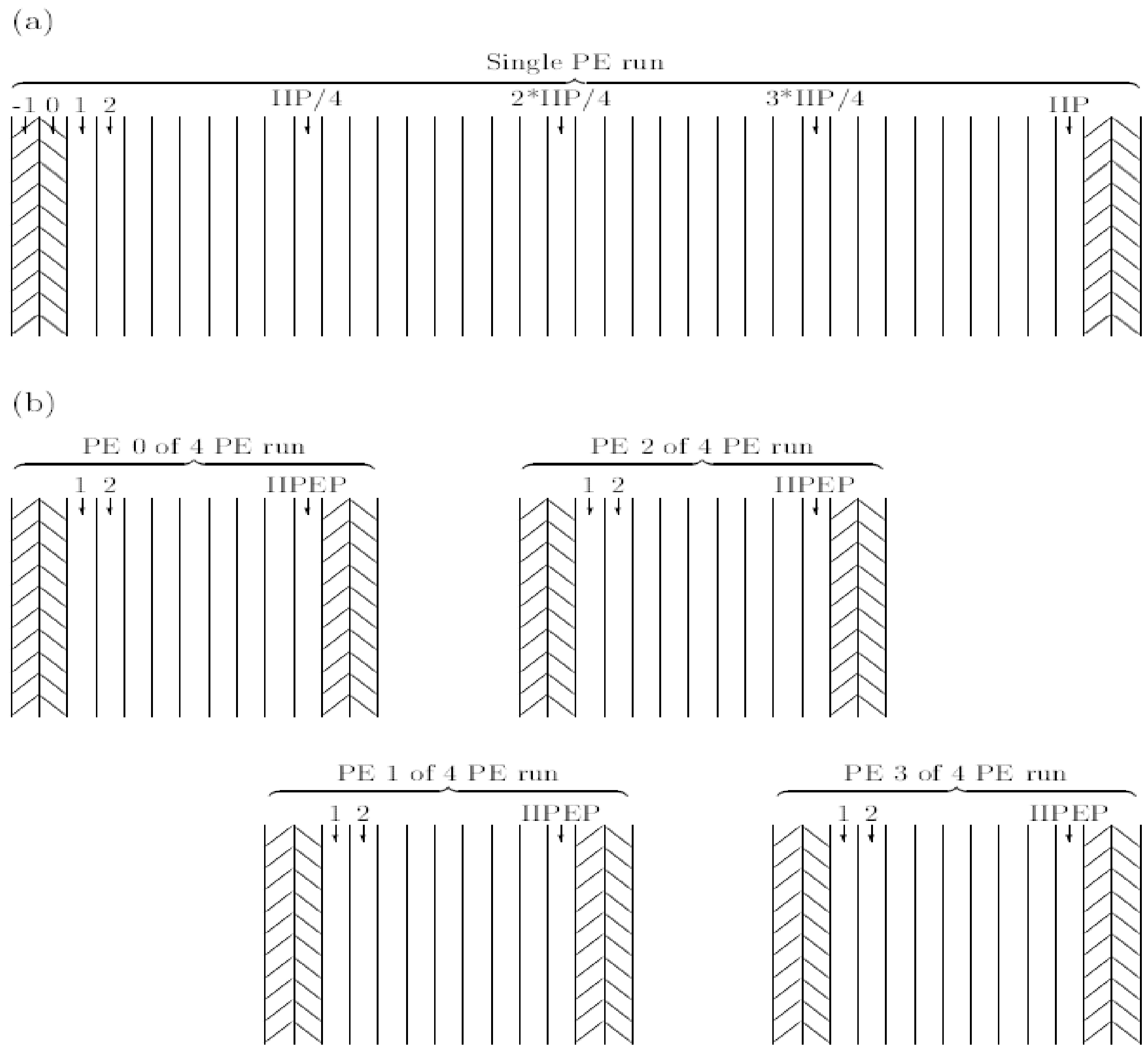
The Decomposed Domain



The Pressure Solver

- Calculation of the pressure term in the system equations requires the solution of a Poisson-like elliptic equation

$$\frac{\partial}{\partial x_i}\left[\rho_s \frac{\partial}{\partial x_i}(p'/\rho_s)\right] = \frac{\partial}{\partial x_i}(\rho_s s_i)$$

where

$$s_i = \delta_{i3}B' - u_j \frac{\partial u_i}{\partial u_j} + \frac{1}{\rho_s}\frac{\partial \tau_{ij}}{\partial x_j} - 2\varepsilon_{ijk}\Omega_j u_k$$

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The Pressure Solver

- This equation had so far been solved via the use of Fourier transforms.
  - Required the use of periodic boundary conditions.
- Using an iterative solver in its place would remove the need for periodic boundary conditions and so enable new science.

A Parallel Iterative Solver

- A good choice of algorithm was found to be the BiConjugate Gradient Stabilized method, or BiCGStab.
- A quick look at the algorithm will highlight what is required to implement it.
- Note that we are solving an equation of the form

$$\mathbf{Ax} = \nabla^2 \mathbf{x} = \mathbf{b}$$

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The BiCGStab Algorithm

1. Compute $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ for an initial guess $\mathbf{x}_0$
2. Initialise $\bar{\mathbf{r}} = \mathbf{r}_0$; $\mathbf{p}_0 = \mathbf{v}_0 = 0$ and $\rho_{-1} = \alpha_0 = \omega_0 = 1$
3. DO i = 1, ITMAX

$$\rho_{i-1} = \bar{\mathbf{r}}^T \bullet \mathbf{r}_{i-1}$$

$$\beta_{i-1} = \left(\frac{\rho_{i-1}}{\rho_{i-2}}\right)\left(\frac{\alpha_{i-1}}{\omega_{i-1}}\right)$$

$$\mathbf{p}_i = \mathbf{r}_{i-1} + \beta_{i-1}\left[\mathbf{p}_{i-1} - \omega_{i-1}\mathbf{v}_{i-1}\right]$$

$$\text{solve}\, \mathbf{M}\hat{\mathbf{p}} = \mathbf{p}_i$$

$$\mathbf{v}_i = \mathbf{A}\hat{\mathbf{p}}$$

The BiCGStab Algorithm

$$\alpha_i = \frac{\rho_{i-1}}{\bar{\mathbf{r}}^T \bullet \mathbf{v}_i}$$

$$\mathbf{s} = \mathbf{r}_{i-1} - \alpha_i \mathbf{v}_i$$

$$\text{solve } \mathbf{M}\hat{\mathbf{s}} = \mathbf{s}$$

$$\mathbf{t} = \mathbf{A}\hat{\mathbf{s}}$$

$$\omega_i = \frac{\mathbf{t}^T \bullet \hat{\mathbf{s}}}{\mathbf{t}^T \bullet \mathbf{t}}$$

$$\mathbf{x}_i = \mathbf{x}_{i-1} + \alpha_i \hat{\mathbf{p}} + \omega_i \hat{\mathbf{s}}$$

$$\mathbf{r}_i = \hat{\mathbf{s}} - \omega_i \mathbf{t}$$

Check for convergence; continue if necessary.

END DO

Calculating Ax=∇^2x

- Assume a 7 point stencil and use the following finite difference relation

$$\nabla^2 \mathbf{f} = \frac{1}{\Delta x^2} f(x+\Delta x, y, z) + \frac{1}{\Delta x^2} f(x-\Delta x, y, z)$$

$$+ \frac{1}{\Delta y^2} f(x, y+\Delta y, z) + \frac{1}{\Delta y^2} f(x, y-\Delta y, z)$$

$$+ \frac{1}{\Delta z^2} f(x, y, z+\Delta z) + \frac{1}{\Delta z^2} f(x, y, z-\Delta z)$$

$$-2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right) f(x, y, z)$$

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Preconditioner

- Use Jacobi method
  - The element-based formula being:

$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j \neq i} a_{ij} x_j^{(k)}\right)$$

Parallel BiCGStab

- Assume the same decomposition along the x-direction.
- There are a number of dot products whose results are required by all processes.
- Calculating expressions of the form $\mathbf{Ax}$ requires halo-exchange between neighbouring processes.
  - Periodic boundary conditions in x and y assumed at the moment.

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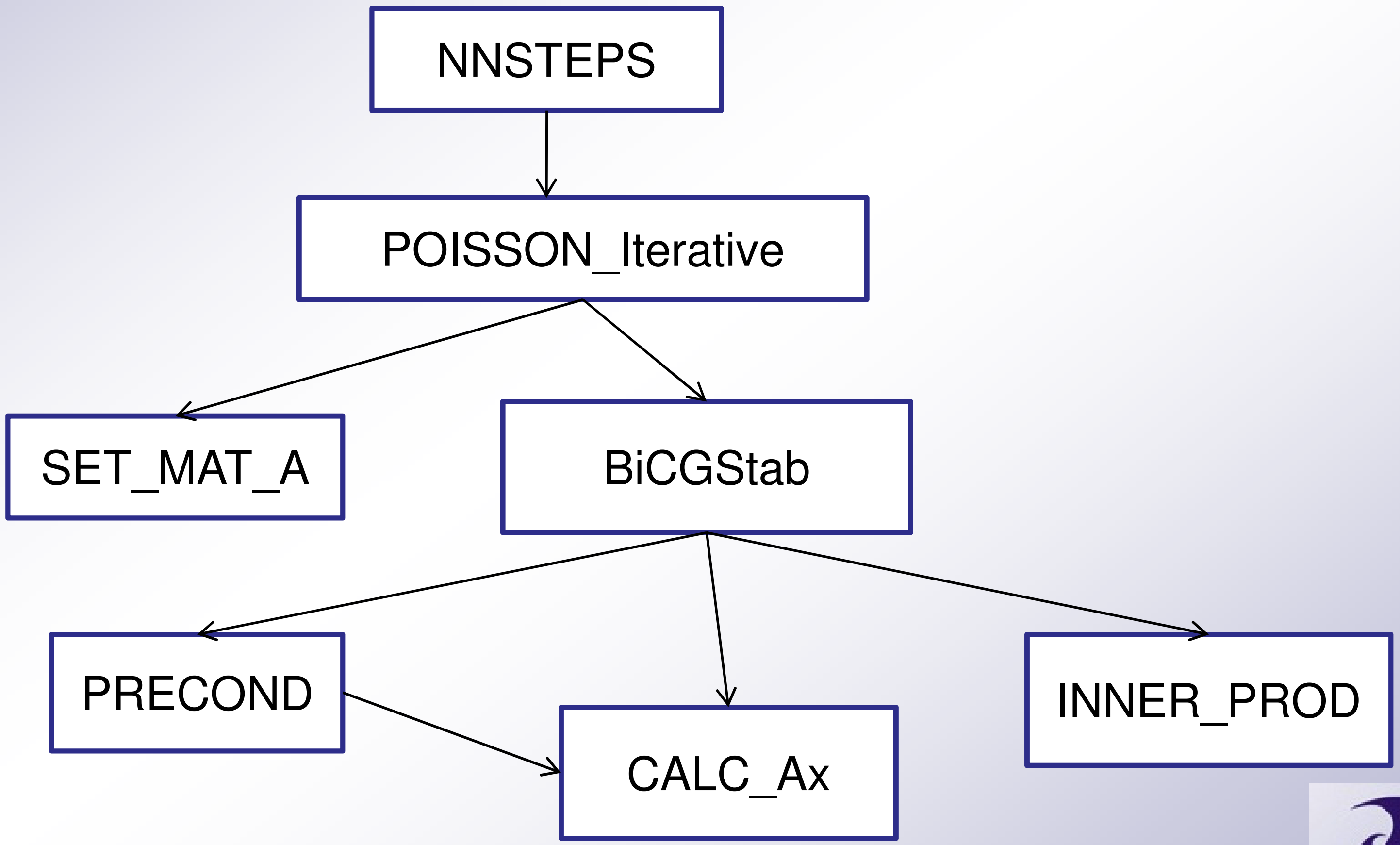
Call Graph for Iterative Solver



Testing the Implementation

- Generate a set of known pressure values, ϕ
- Calculate the input source terms using

  $$\mathbf{f} = \nabla^2 \phi$$
- Use the iterative solver with $\mathbf{f}$ as the input.
- Does it give us back our original set of pressure values, ϕ ?

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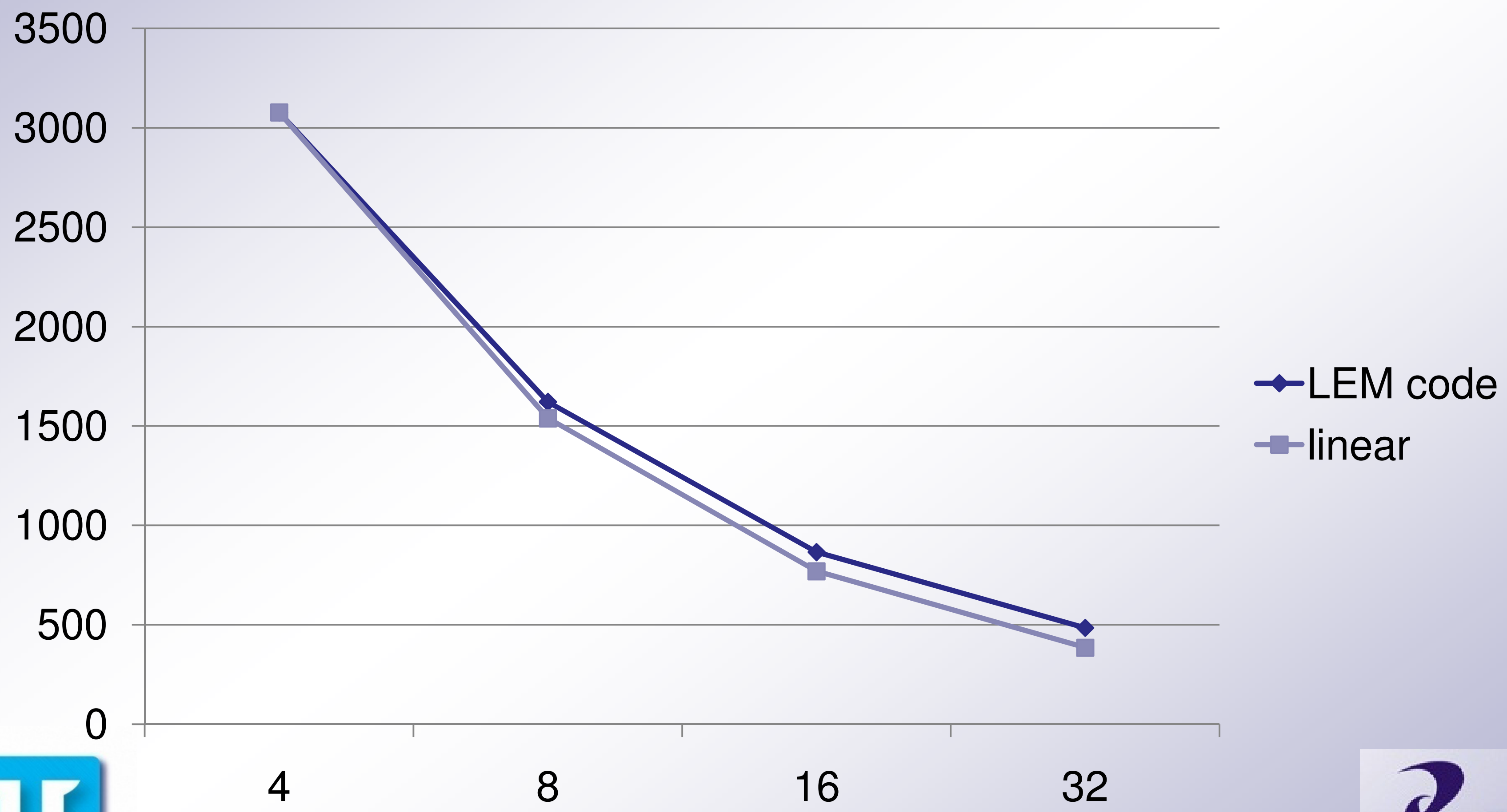
Optimising the Implementation

- Used CrayPat and output from -Minfo/-Mneginfo PGI compiler flags
  - Modified code to improve cache re-use
  - Sometimes compiler did the wrong thing
  - Improved the communication...

GCOM, MPL or MPI?

- Existing communication in the code is very inefficient.
- I used GCOM initially...
- ...but to give better communication performance, now call the intermediate MPL library layer.

Wot, no scaling graph?



Potential Future Work

- Move to a 2D domain decomposition
- Improve the communication in the rest of the code
- Modify the memory use

Questions?