NEPTUNE: Numerical Analysis

Sue Thorne (PI) and Tyrone Rees (Co-I)

Work Package Themes

Preconditioners for Plasma Modelling

Time Advance Techniques for Plasma Modelling

Coupling of Continuum (Fluid) and Particle Models for Plasma Modelling

State-of-the-art Solution Continuation Techniques

Adjoint Methods for Fusion

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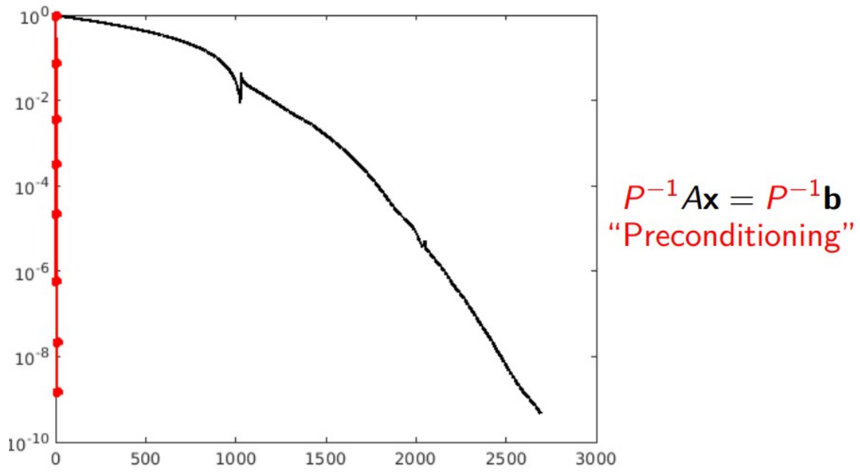
Preconditioners for Plasma

Continuation of Mathematical Support Project
- Build on earlier deliverables

The proxyapp will have identified the most promising candidate preconditioner for NEPTUNE, and we will:
- Implement this in a documented library (probably PETSc-based) to be called by other NEPTUNE software
- Investigate preconditioning methods for coupled elliptic and parabolic systems.



Deliverables
- Update the three technical reports previously delivered on preconditioning **(31/3/23 & 14/2/24)**
- Develop a technical specification for the software library **(31/3/23)**
- Identify a block preconditioner for implementation **(14/2/24)**
- Develop library and associated docs **(31/3/23 & 14/2/24)**

Dependencies
- Agreed technical specification with Nektar++ team and other interested parties

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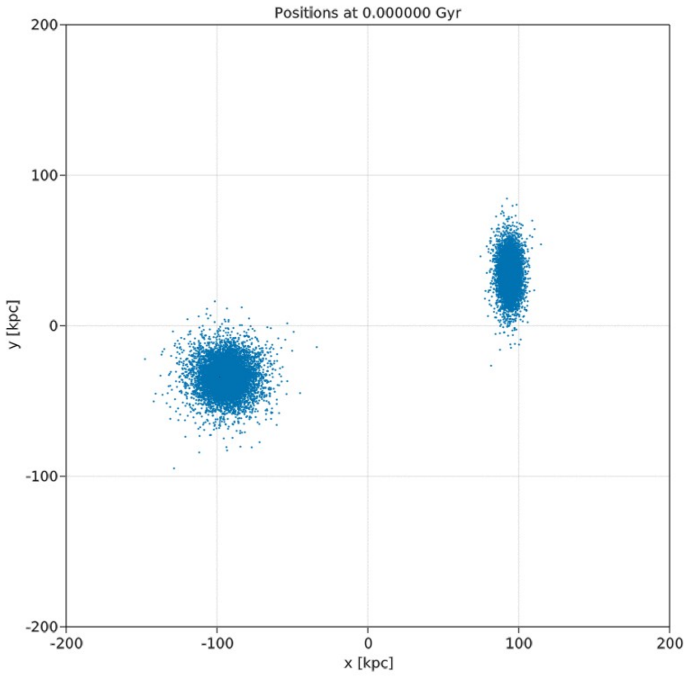
Time Advance Techniques

Continuation of Mathematical Support Project

- Build on earlier deliverables

The proxyapp will have identified the most promising candidate time-stepping for NEPTUNE, and we will:

- Implement this in a documented library (probably PETSc-based) to be called by other NEPTUNE software



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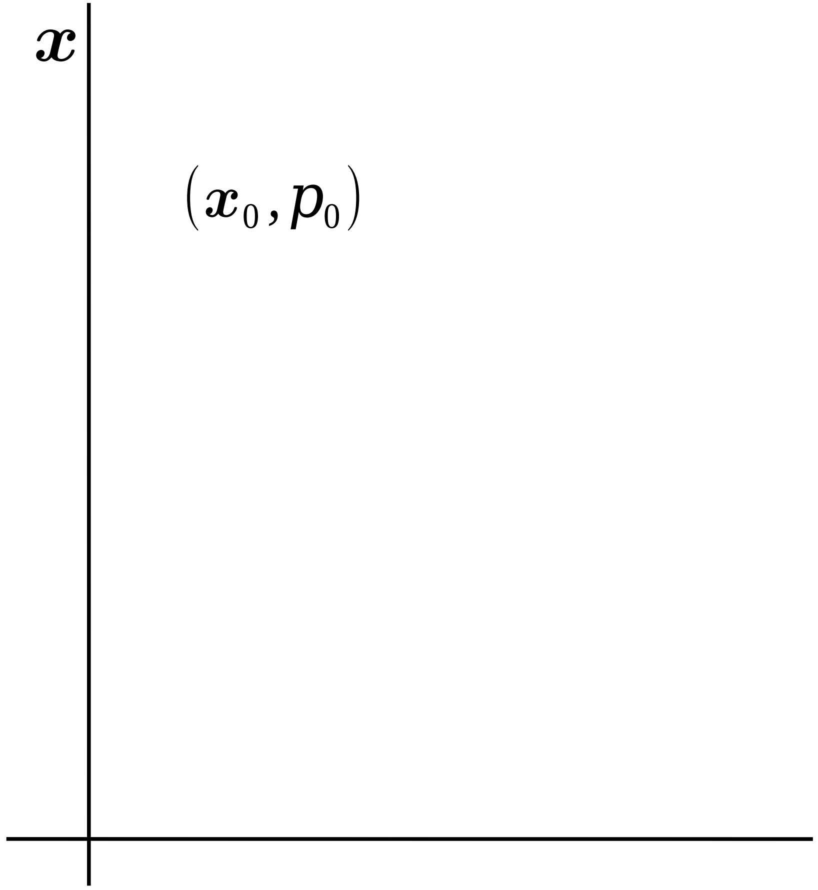
State-of-the-art Solution Continuation Techniques

Find solutions to the nonlinear equations

as a function of the real parameter, .

Given a known solution , we can continue it by computing a curve of solutions that passes through .



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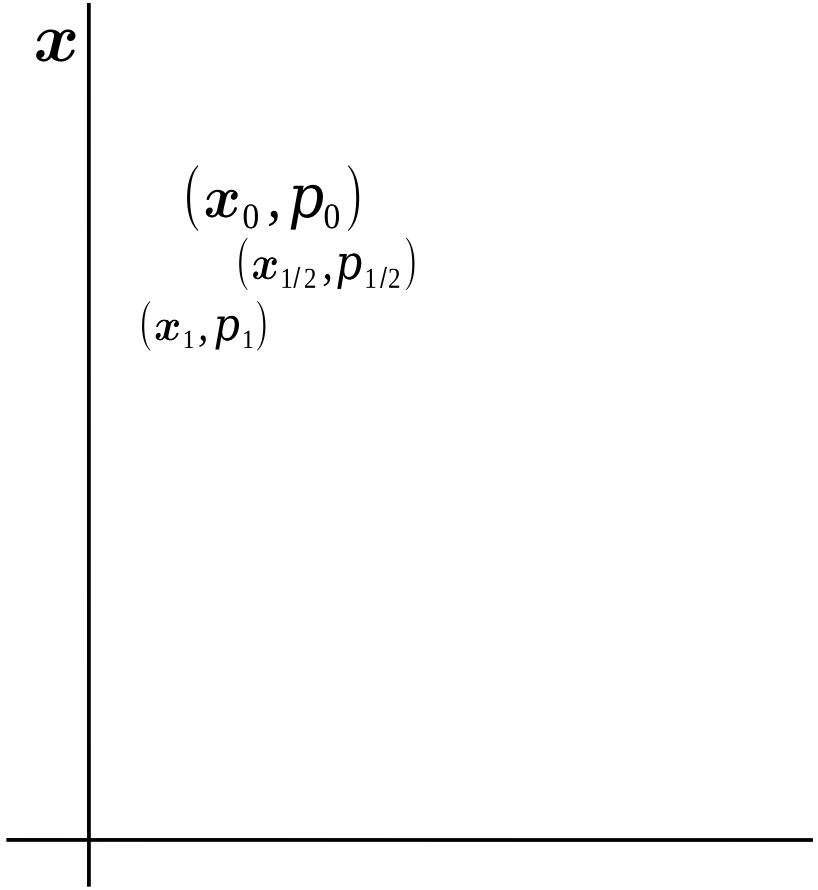
Predictor-Corrector methods

These methods make a (cheap) prediction of the next point, and then use a more expensive method to correct the guess to lie on the solution curve.



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Predictor-Corrector methods

Predictors

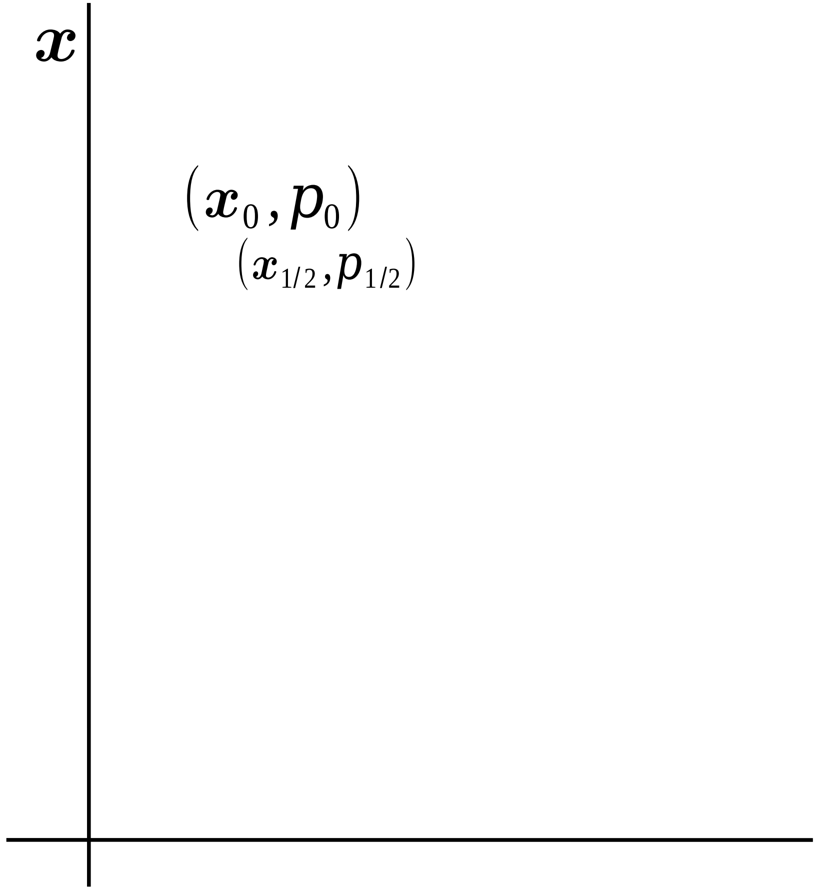
Natural predictor
Based on the naïve choice of

For some small step size .

First order predictor
Uses derivative information

Where is (an approximation to) the tangent at

….



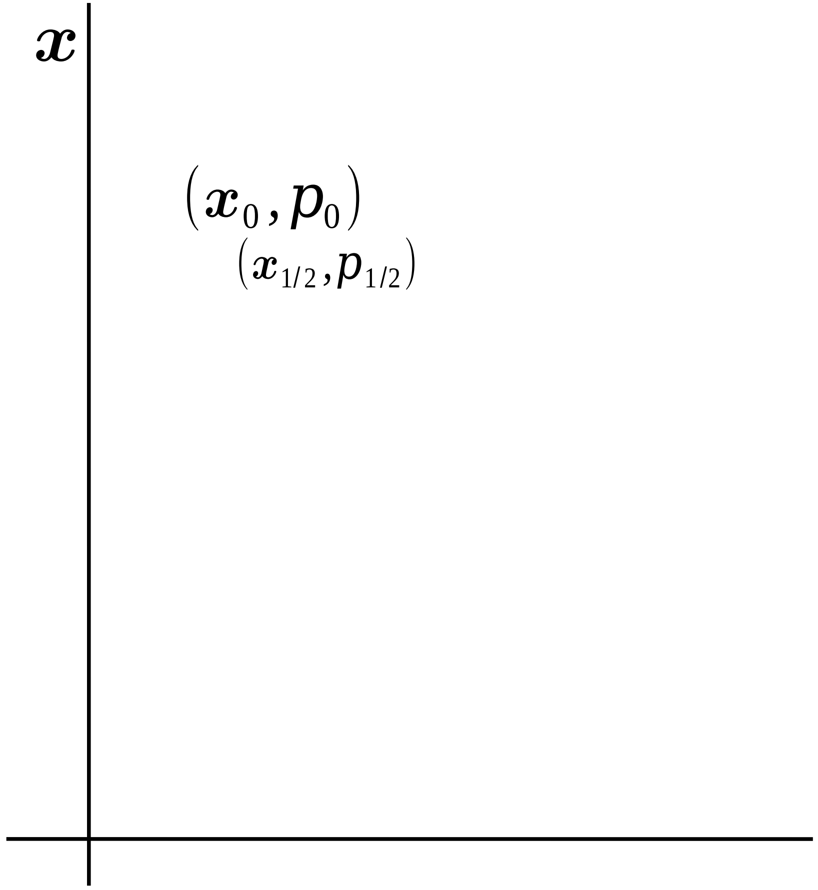
Predictor-Corrector methods

Predictors

Polynomial predictor
Uses least-squares regression to fit a polynomial of degree to the last solution vectors (), and uses this to generate the prediction step.

Multiple predictor
Use multiple predictors with different steps sizes, and choose the largest step with sufficient decrease of the corrector.

Can be more robust, especially in problems from PDEs.



Predictor-Corrector methods

Correctors

Newton's Method

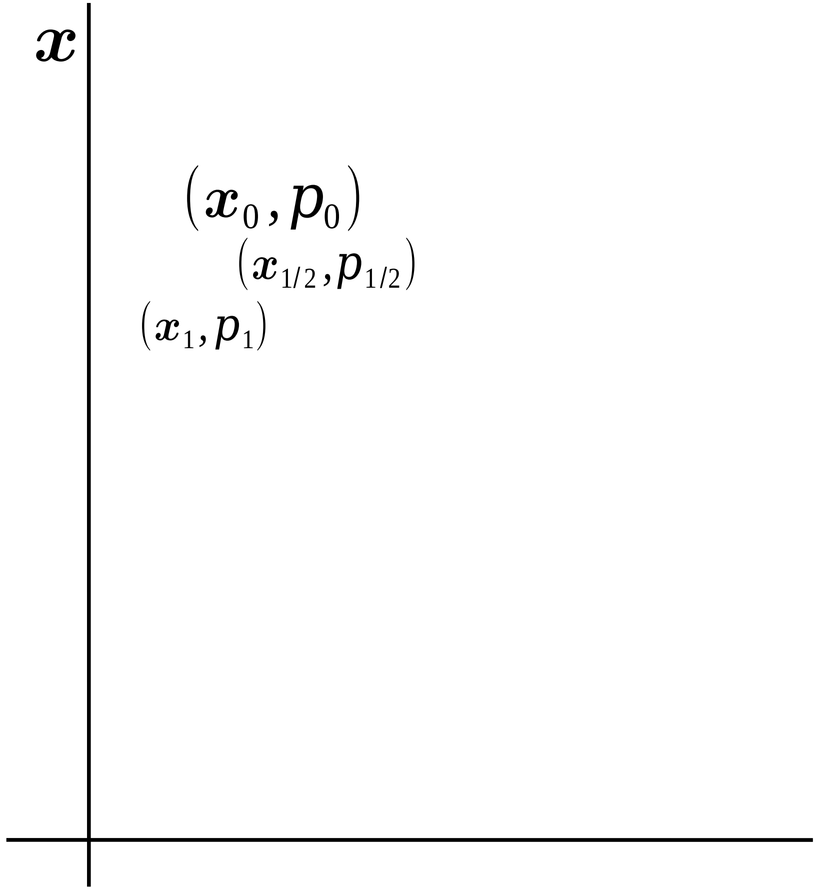
If solving , Newton's method takes the form:

Problem: The Jacobian of is non-square, so can't be inverted.

Solution: Use the Moore-Penrose pseudo-inverse,

This is equivalent to solving the NLLS problem

y using a Gauss-Newton method.



Predictor-Corrector methods

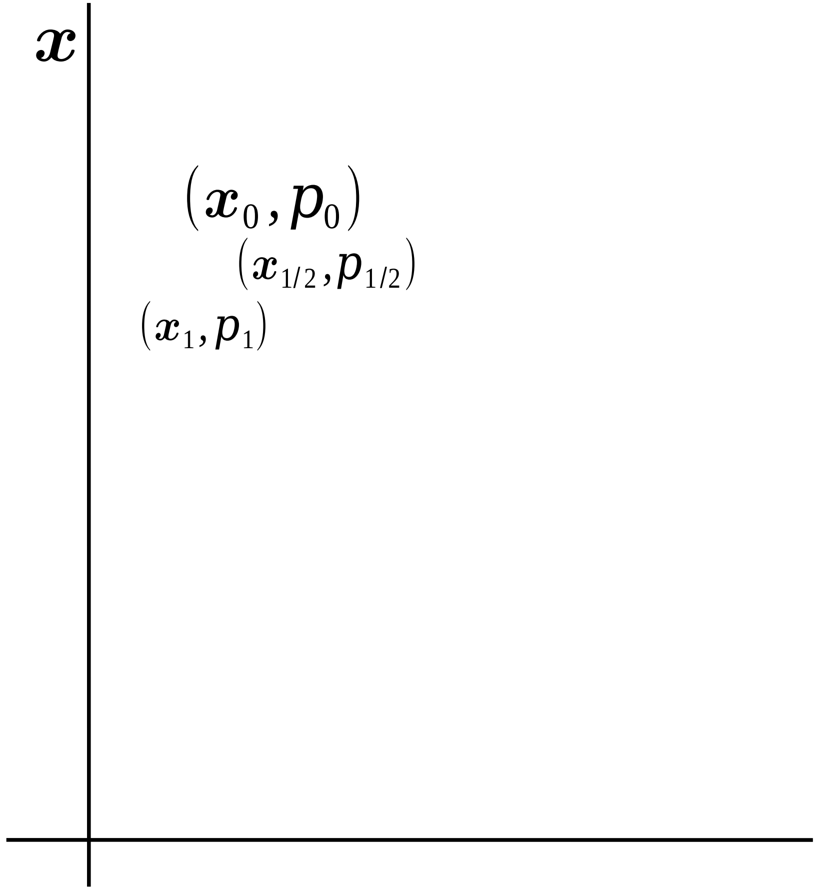
Correctors

Pseudoarclength continuation

We can also add constraints to the equation, to make the Jacobian invertible. For example, solve

where is the pseudoarclength, an approximation of the arclength in the tangent space of the curve.

The Newton step in this case requires the solution of a square matrix:

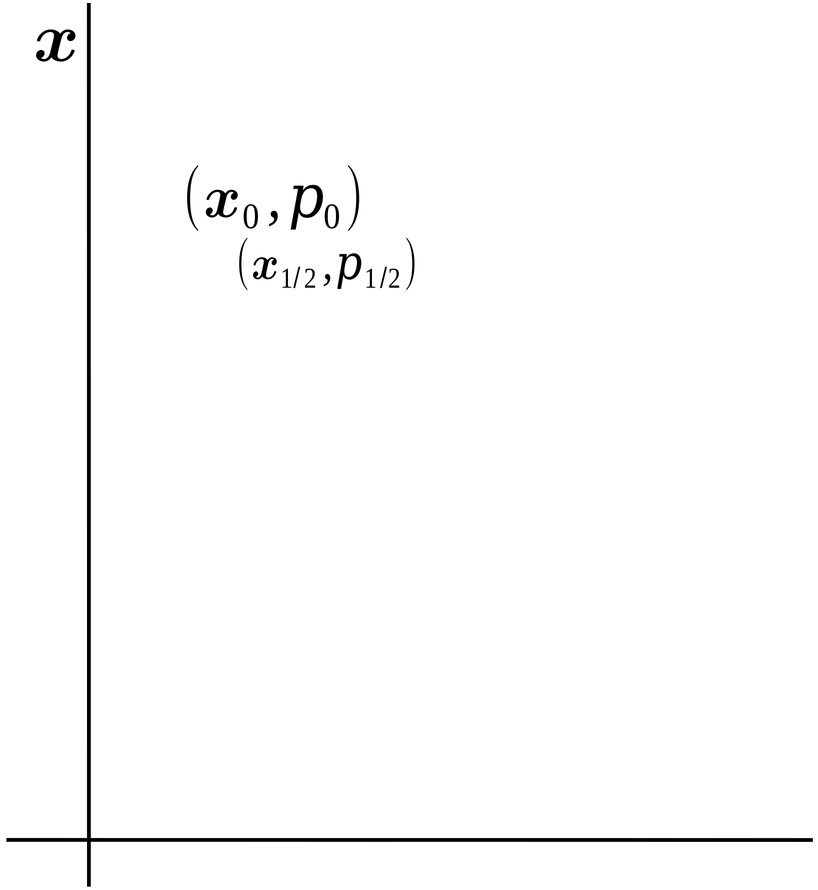


Predictor-Corrector methods

Step length

The predictor gives a direction, but we need to specify a length of step to take in that direction. If the region is smooth, a large step can be taken. If there is lots going on, we need to take a smaller step.

Various adaptive strategies have been proposed, which we will explore.

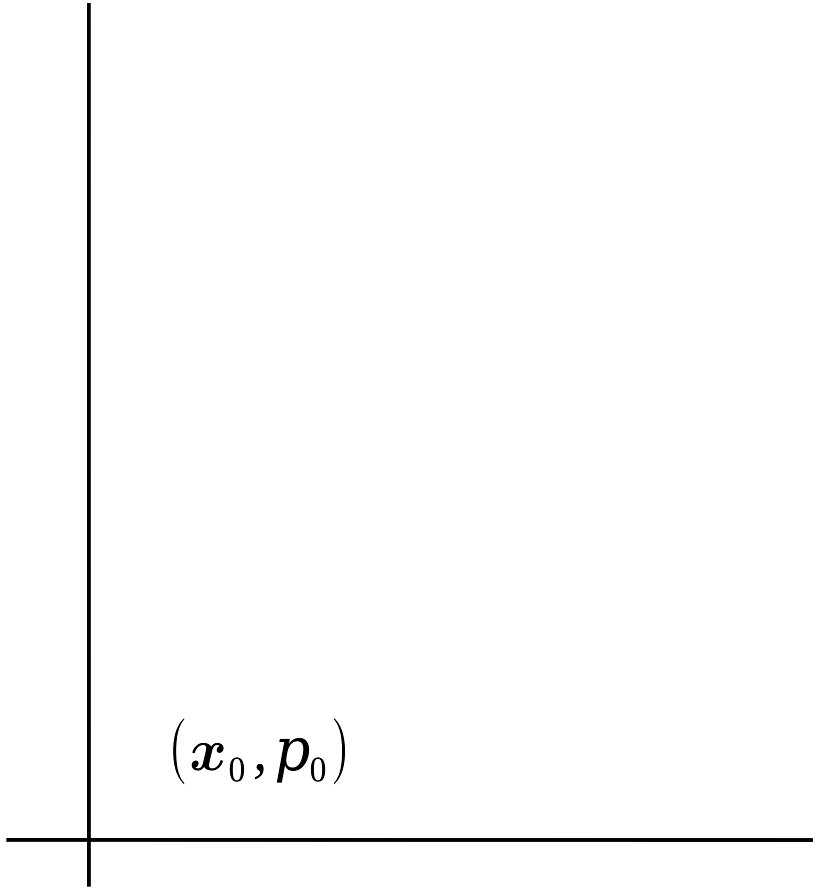


Predictor-Corrector methods

Special points

Points, such as turning points or bifurcation points, often need to be identified accurately.

Some of the methods discussed previously are more robust to such features than others.

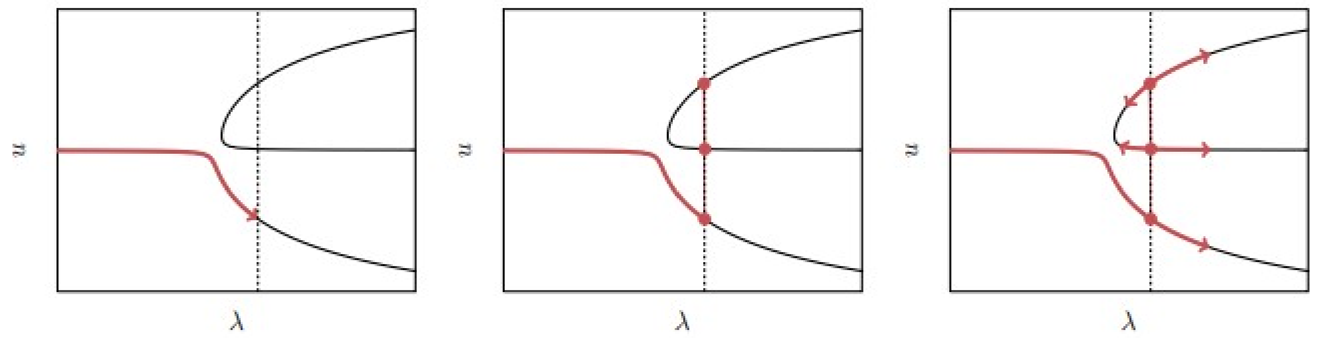


Predictor-Corrector methods

Deflation

Deflation techniques [†] allow us to find multiple branches, and can be applied in case where the bifurcation diagram is disconnected.

These work by modifying the nonlinear system so that Newton's method does not converge to a known root.



(a) Initial continuation (b) Apply deflation (c) Continuation of branches

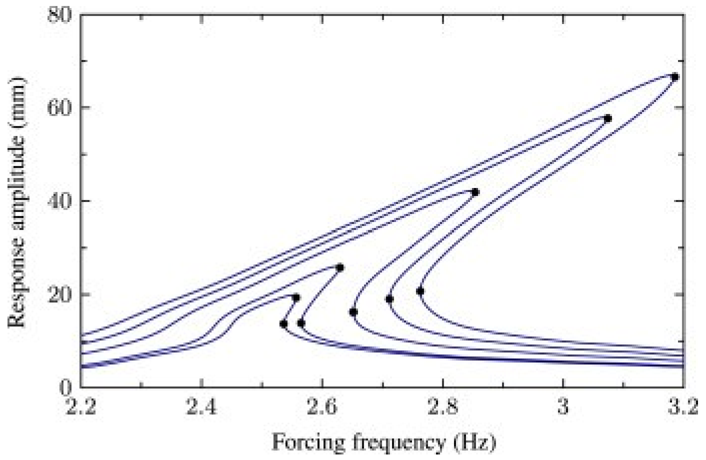
[†] Farrell, Beentjes and Birkisson 2016 https://arxiv.org/abs/1603.00809v1

State-of-the-art Solution Continuation Techniques

Investigate the state of the art in

- Predictor techniques
- Corrector methods
    - Linear solver and other algebraic considerations
- Step size selection
- Critical point identification

as applied in a HPC/Exascale environment applied to spectral element codes for plasma modelling.



Deliverables

- Report summarising literature and software available for continutation methods. **(31/7/2023)**
- Proxyapp implementing a suitable technique on a test problem relevant to plasma modelling. **(14/2/2024)**
- Report/presentation summarizing proxyapp test results. **(14/2/2024)**

Dependencies

- Success requires at least one representative problem for which solution continuation techniques will be applied to in NEPTUNE, with particular reference to the needs of the grant holders working in UQ.

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Coupling of Continuum (Fluid) and Particle Models for Plasma Modelling

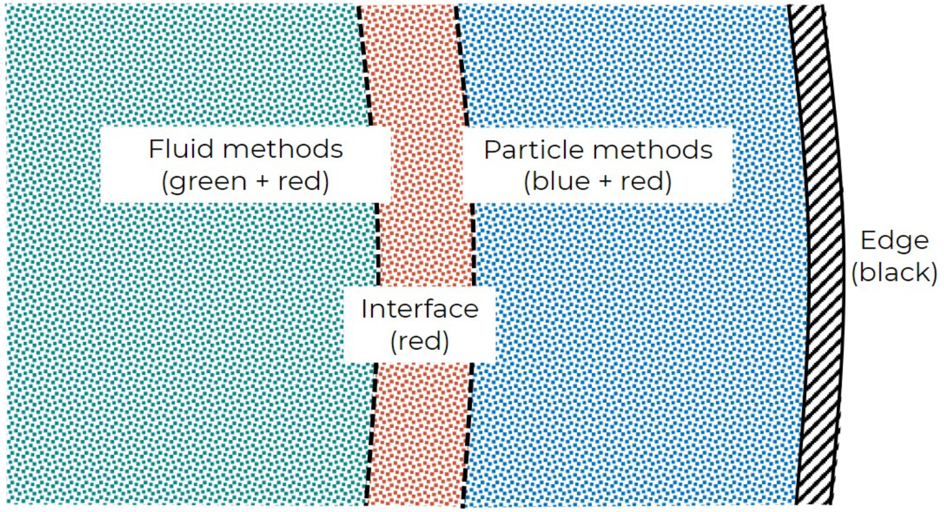
Continuation of Mathematical Support Project

- Build on earlier deliverables

Three main coupling methods

- Kinetic-Diffusion Monte Carlo Method (KDMC)
  - Each MC particle alternates between fluid and kinetic actions
- Micro-Macro Hybrid Method (mMH)

  - Significant changes to NEPTUNE Programme required
- Spatial Hybridization (SpH)
  - Separation of concerns
  - Existing libraries identified: CWIPI, MUI and preCICE



Spatial Hybridization (SpH) Approach

Deliverables (31/3/2023)

- Software module for SpH method
  - Linking Nektar++ fluid and particle approaches
  - Allow investigation of the interface: Location? Size?
- Results from benchmark tests
- Updated reports

Dependencies

- Agreed technical specification
- Provision of appropriate fluid and particle codes

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Adjoint Methods for Fusion

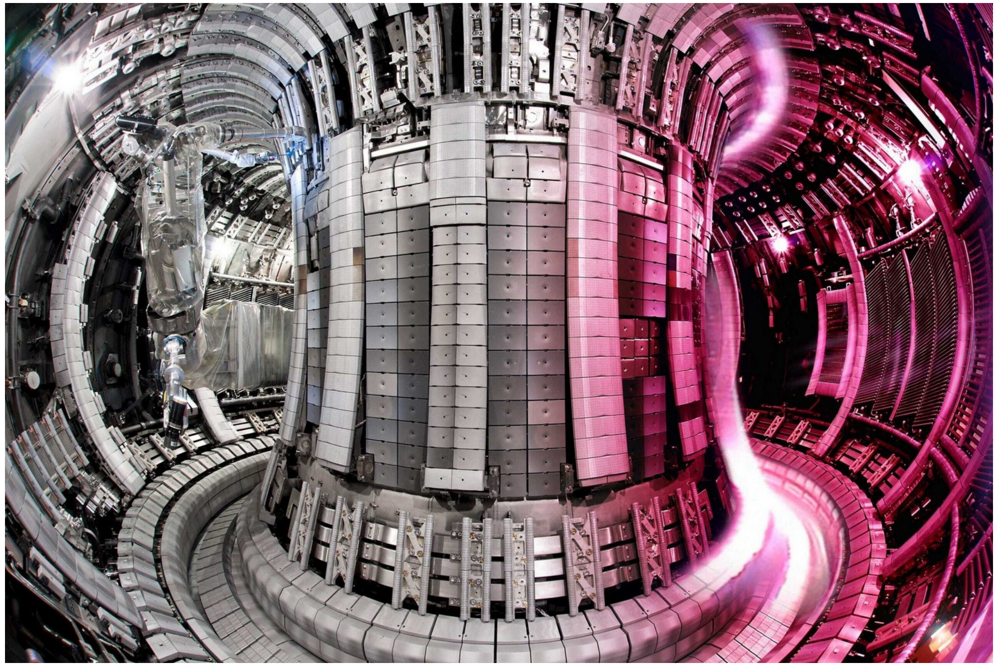
Build on knowledge developed within project from FARSCAPE2

- Derive and implement adjoint for ideal MHD, Grad-Shafranov equilibrium
- Use adjoint model to study stability/sensitivity and compare to literature
- Ubaid Qadri and Daniel Ward

Identify state-of-the-art algorithms for generating and solving adjoint equations, and their applicability to plasma modelling, e.g., sensitivity analysis, optimization

- For sensitivity analysis, variational form is used and mean value theorem applied to write linear form → adjoint problem

Identify algorithm and develop proxyapp



Deliverables

- Report identifying current state-of-the-art algorithms for generating and solving adjoint equations that may be suitable for HPC/Exascale implementation particularly in the context of spectral element code for plasma modelling (31/7/23)
- Proxyapp and benchmark results (14/2/24)

Dependencies

- Following literature and software review, feedback on areas to concentrate on

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